Cosmological Dynamics, Statistics and Numerical Techniques of $f(R)$ Gravity

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Abstract

Inflation is a much discussed topic within the field of cosmology; it represents a time in the history of the Universe where a very rapid, exponential expansion was taking place. This expansion is needed in order for the currently used Big Bang model to fit with what we observe today; however the nature of this inflation is still not well understood. Among the theories of how inflation starts, evolves and ends, $f(R)$ gravity is the one we will focus on in this thesis. The most attractive trait of $f(R)$ gravity is that it can explain the accelerated expansion without the need of introducing exotic, new particles and/or energies into the Universe, such as dark energy and dark matter. During the research in this thesis of $f(R)$ gravities we came across what seems to be an as of yet unappreciated problem that arises when we perform a so-called conformal transformation between the Jordan and Einstein frames. If we are not careful, the conformal transformation can tangle our coordinates, so that we might produce errors in codes that have not accounted for this entanglement. This understanding allowed us to produce a paper titled "Gauge Issues in Extended Gravity and $f(R)$ Cosmology", published in the Journal of Cosmology and Astroparticle Physics Issue 04, 2012. From this spawned a new direction of the research, to modify an existing Boltzmann code in order to fully safeguard against these problems. After reviewing the biggest Boltzmann codes, the choice fell to either CLASS or CAMB, where we chose CAMB due to the fact that Fortran is a much more familiar language than C, even though it could be argued that CLASS is the more readily modifiable, while remaining stable, program. The process of modifying CAMB is almost complete at this point; however, it is not yet in a state suitable for presentation. The thesis also performs an analysis of the so-called "non-Gaussianity" parameter f_{NL}, CMB power spectrum and CMB bispectrum for a specific $f(R)$ model, in order to probe its viability, and to demonstrate the techniques we will apply to more general models.

Acknowledgments

I would like to start with thanking my supervisor Iain A. Brown, for introducing me to the exciting field of extended gravity, and for being a reliable and very helpful supervisor for the myriad of questions I've had throughout this research. I also want to thank my co-supervisor Frode Hansen for first mentioning Iain as a potential supervisor, and for otherwise having been a great teacher in the previous years.

I also want to thank my girlfriend Isabel Gulliksen, who've been an immense support when things got rough, and who has been very understanding of the long hours I've been busy for the latter part of my research.

Lastly I want to thank all the other students in Stjernekjelleren, who've made the two years working on my masters a very pleasent experience, everyone who play on the Astrostars football team for some much needed football exercise after a long week of work, and of course my family, for having been supportive of me for all these years.

Contents

Chapter 1

Introduction

In this thesis we will discuss $f(R)$ models in cosmology and develop techniques to analyze CMB non-Gaussianity induced by such models. The techniques will be able to solve a wide range of modified gravity models, not limited to $f(R)$ models. In this thesis we will only utilize $f(R)$ theories in our examples, this is however only as a test case. We apply our developed techniques to modify an existing Boltzmann code, CAMB.

Here follows a short outline of the thesis; In Chapter 1 I have a short introduction to my entire thesis, followed by all the preliminaries we need to know for further research in Chapter 2. In Chapter 3 I give a general introduction to $f(R)$ gravity theories, while in Chapter 4 I discuss the statistics of an arbitrary $f(R)$ gravity model. In Chapter 5 we take a look at the gauge-issues that exist when cosmologists wish to transform between the Einstein and Jordan frame, or more generally when anyone wishes to perform any kind of conformal transformation. This chapter covers our paper "Gauge Issues in Extended Gravity and f(R) cosmology" [1]. In Chapter 6 we start using what we learned from the previous Chapters in order to modify CAMB for extended gravity theories. In Chapter 7 we provide the results from Chapters 3-6, and we finish in Chapter 8 with conclusions of the various results.

My thesis has undergone quite a few changes from when I first started out, and was originally not supposed to be what is outlined above. The original goal would be to analyze a specific $f(R)$ gravity theory in order to find what magnitude of non-Gaussianity $f_{\rm NL}$ it would provide. We have constraints on the value of $f_{\rm NL}$ from observations, and these constraints will be improved in the near future once data from the Planck satellite is available. This non-linearity parameter $f_{\rm NL}$ will allow us to rule out or reaffirm various $f(R)$ theories. All of this however, was covered in detail in a paper by Shinji Tsujikawa and Antonio De Felice [2], which emerged shortly after we first approached the topic, and what was to be my entire thesis has now been reduced to Chapter 3.

However, that paper did not stop me from wanting to work on $f(R)$ gravity theories. They represent a very fascinating, and in my mind smart, way of describing the inflationary epoch without having to introduce exotic particles and energies such as dark matter and dark energy[1]. With some luck a summer project where we analyzed

[1] These dark quantities are called so because they represent something unknown that we cannot

the Einstein and Jordan frame pushed us onwards to a new goal for this thesis, which is what is outlined above.

Next I'll supply some notes that will be important for the entire thesis.

1.1 Notations and Miscellaneous

This section contains a listing of the different notations we'll be using throughout the thesis, as well as other techniques that may not be obvious to the reader.

1.1.1 Conformal Time

We'll use what is known as the **conformal time** η rather then the traditional cosmic time t,[2] defined as

$$\eta \equiv \int_0^t \frac{dt'}{a(t')}. \tag{1.1}$$

The conformal time represents the co-moving distance that light could have traveled since a time $t = t'$ [3], η therefore represent the size of the Universe today, and things separated by a distance greater than η are not causally connected. More on this in §2.6.

1.1.2 Einstein Summation Convention

Throughout this paper we will be using what is known as the Einstein summation convention. It tells us to sum over all possible values of indices that appear both as super- and subscripts,

$$g_{\alpha\beta}R^{\alpha} = \sum_{a=0}^{3} g_{a\beta}R^{a}. \tag{1.2}$$

Note that *Latin* letters represent the spatial part, and the sum shall only go from $a = 1, ..., 3$, whereas *Greek* characters include the time part, and should sum from $a = 0, ..., 3$. This notation makes the complicated math of General Relativity much more manageable.

observe directly, yet. They are however needed to unify theory with the observed nature of the Universe, unless we use extended gravity theories.

[2] We can easily convert equations in the literature given in cosmic time to conformal time with the relation $dt = ad\eta$.

1.1.3 Derivatives

In general we also have the following derivative notations for a scalar A and tensor F:

$$\begin{aligned} \frac{dA}{d\eta} &= \dot{A}, \quad \frac{\partial A}{\partial x} = A_{,x}, \ \frac{\partial^2 A}{\partial x^2} = A_{,xx} \\ \partial_i A = \frac{\partial A}{\partial x^i}&, \quad \nabla^2 A = \partial_i \partial^i A \\ \Box = \nabla^\mu \nabla_\mu&, \quad \nabla_\mu F_\nu = \partial_\mu F_\nu - \Gamma^\sigma_{\mu\nu} F_\sigma \\ \partial_{(i} F_{j)} = \partial_i F_j + \partial_j F_i&, \quad \partial_{[i} F_{j]} = \partial_i F_j - \partial_j F_i, \end{aligned}$$

where $\Gamma^\sigma_{\mu\nu}$ is the Christoffel symbol – more on this in §2.4.3 – and x_i is the i'th component of the vector $\mathbf{x} = (\eta, x, y, z)$.

1.1.4 Other Conventions

We will be working in certain specific units throughout this thesis in order to simplify the majority of the equations. We will be working in units where the speed of light $c = 1$, with a quantity κ given by $\kappa^2 = 8\pi G$ where G is Newton's gravitational constant, and typically with no cosmological constant $\Lambda = 0$. We employ a metric signature (-+++) and the Ricci tensor $R_{\mu\nu} = R^\alpha_{\alpha\mu\nu} = \Gamma^\alpha_{\mu\nu,\alpha} + ...$ – more on this Ricci tensor in §2.4.3.

Chapter 2

Preliminaries

2.1 The Concept of Modern Cosmology

Cosmology is in general the study of everything. We attempt to understand how the universe first began, how it evolves, what it looks like and what size it has, how old it is, and of course, how it will all end. In the two next sections several terms will crop up that will be further explained in the following sections.

The field of cosmology is built upon one underlying principle, **the Copernican principle**, also known as the cosmological principle. It tells us that no places in the Universe is special[1], and that one point in space should be able to represent every other point in the Universe. This is also the basis for the Big Bang cosmology.

A lot of this chapter has been inspired by Sean M. Carroll's "Spacetime and Geometry" [4], Øyvind Grøn's "Einstein's General Theory of Relativity" [5], Andrew Liddle's "Introduction to Modern Cosmology" [6], Scott Dodelson's "Modern Cosmology" [3] and lecture notes by local Professor Øystein Elgarøy [7], as well as various other minor sources.

2.2 A Very Short History of Everything

The current Big Bang theory of cosmology assumes that the Universe started out from one singularity where all the mass of the Universe was collected at a time $t = 0$. The laws of physics as we know them today allow us to describe the Universe as far back in time as the end of the Planck era. The Planck era was a time when we suspect the Universe was filled with relativistic elementary particles such as quarks, leptons, gauge bosons and possibly the Higgs boson[2], to do any actual calculations in this era we would need a new theory of quantum gravity. The Planck era lasted from the Big Bang until a Planck time later, where from Quantum Physics and Heisenberg's uncertainty principle

[1] In striking contrast to long held beliefs that the Earth was the center of Universe.

[2] CERN are confident that they will find the Higgs boson soon at the time of writing; it will remain to be seen if they actually do.

we can construct the Planck time as

$$t_{Pl} = \frac{\hbar}{M_{Pl}c^2} = \sqrt{\frac{\hbar G}{c^3}} = 5.4 \cdot 10^{-44} \text{ s}, \tag{2.1}$$

where M_{Pl} is the Planck mass[3], $\hbar$ is the Planck constant and G is the Gravitational constant. At the Planck time, we can find the radius of the observable Universe to be of the Planck length $l_{Pl} = ct_{Pl} = 1.6 \cdot 10^{-35}$ m and with a temperature of $T_{Pl} = 1.5 \cdot 10^{32}$ K.

After the Planck era, we immediately enter the inflationary era, starting at $t = 10^{-43}$ s after BB, and lasting until $t = 10^{-33}$ s. During this very short period the Universe went through a very rapid exponential expansion, increasing the size of the Universe by a factor of 10^{43}. In a matter of 10^{-33} seconds the entire observable Universe went from being on a sub-nuclear scale to an astronomical scale! As well as expanding the Universe at an exponential rate, inflation is a solution to other curious problems with the Big Bang theory; we'll return for a more detailed look at inflation in §2.7. As the size of the Universe increased, the temperature decreased. Soon the temperature had dropped sufficiently far enough to allow elementary particles in the Universe to start forming larger nucleus, and eventually atoms.

Shortly after inflation ended, when the Universe was about one second old, what we call Big Bang Nucleosynthesis started. This is the process where the first protons and neutrons met and formed nucleons; however due to the high temperature of the Universe and the abundance of photons, the electrons still remained free. Whenever an electron attempted to join with a photon and neutron to form a stable atom, it would be kicked straight out by a passing photon. Therefore the Universe remained in a state where it was filled with an ionized gas, until the temperature dropped far enough to initialize decoupling[4].

Decoupling occurred about 300 000 years after the Big Bang, when the temperature of the Universe had dropped down to about 2700 K,[5] allowing electrons to bind with protons and neutrons without instantly being excited again. After this had been going on for a little while, almost all the electrons in the Universe had settled down into the ground state of the atoms, and for the first time, photons could travel freely through space. This event turned the Universe from an opaque gas, to being completely transparent. The photons we detect today have been traveling for a long time, and have reduced their temperature from 3000 K to about 2.7 K due to the expansion of the Universe, which is equivalent to their wavelengths having been redshifted so that they now are only observed in the microwave region of the electromagnetic spectrum. This is

[3]For the majority of this thesis we will be working with the reduced Planck mass $m_{Pl} = (8\pi)^{-1/2} M_{Pl}$.

[4]As decoupling is a general term that can be used for several epochs in the Universe and in general, the term "Recombination" is often used for this event. However, as this is the first time protons, neutrons and electrons combined the first atoms, the "Re"-part is not a proper term to use, and will therefore not be used in this thesis.

[5]This is an average temperature, meaning that there are countless photons still around with a much higher temperature. This is the reason why decoupling didn't take place the moment the temperature of the Universe dropped down below the binding energy of electrons.

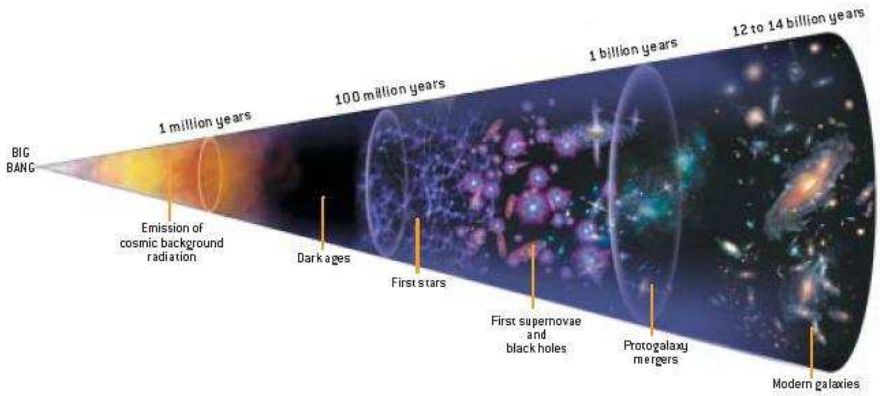

Figure 2.1: Sketch of the evolution of the Universe, courtesy of Scientific American.

the origin of the Cosmic Microwave Background (CMB) radiation, a snapshot of what the Universe looked like 300 000 years ago.

After this event, the Universe didn't undergo any major changes for quite some time. It continued to expand, cool down, and the gas cloud of newly formed atoms were allowed to interact with each other, clustering together thanks to gravity, and creating even stronger gravitationally bound gas clouds. Eventually some of these gas clouds became so dense that the gravity of the gas itself caused it to collapse inwards, increasing the density and temperature of the gas cloud. When the pressure and density were sufficiently high, new nuclear reactions started, and the very first stars of the Universe were formed. These stars started sending out new, fresh photons, with energy high enough to ionize the rest of the gas in the Universe. This event, called re-ionization, returned the gasses of the Universe closer to their previous state, and is generally considered to be a problem for observational astronomers when they are observing the moment of decoupling. However, the features reionization has on the CMB can help break degeneracies in the observed parameters that we would otherwise be left with.

From here on in, more stars were formed, stars died after having formed the heavier elements, and this seeded the Universe with the elements needed to form the first planets and other massive objects. These supernovae also play a big part for observational astronomers, especially when they are to gauge distances in the Universe. This concludes our brief overview of the history of the Universe. How will it continue from here? That is among the many questions modern cosmologists are attempting to answer.

2.3 Modern Cosmology in a Nutshell

Let's continue with an intuitive way of looking at the field of cosmology. Imagine the universe as consisting of a complicated and complex **spacetime** surface, in order to simulate this we have a simplified model of a flat and nice-looking spacetime, which is suitable to explain most of our observations. But then, in order to meet the additional requirements set by more extensive surveys such as the **CMB**, we add **perturbations** to our flat spacetime, and we will have gotten a model that is closer to the real deal, but still relatively nice and easy to use in simulations. This process is illustrated in Figure 2.2.

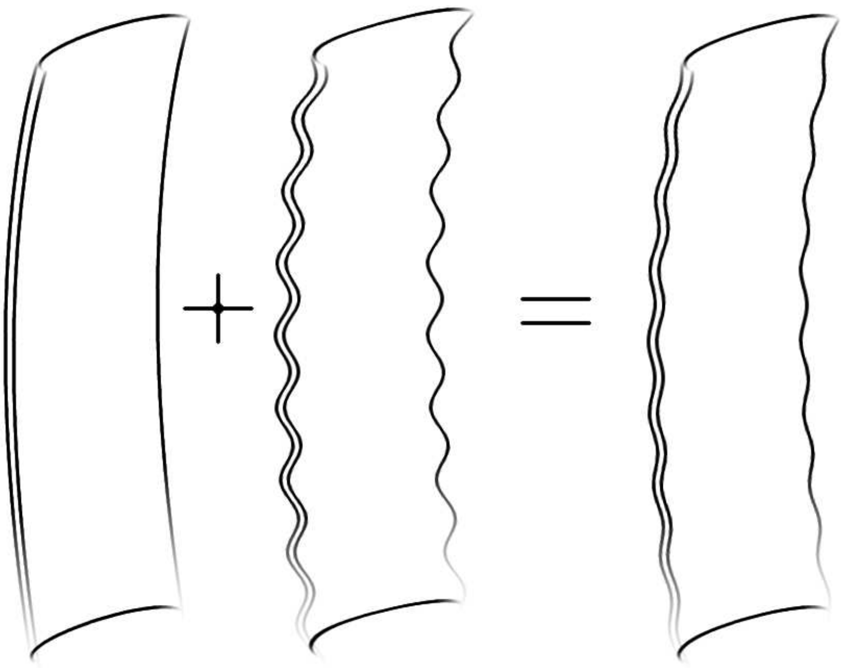

Figure 2.2: The real spacetime of our universe is represented as a messy shape on the right. We attempt to approximate the real universe by using a simple cosmological model, and add perturbations to the smooth surface to get closer to the actual reality.

Unfortunately we don't work with just one kind of **metric** (representation of our spacetime), but rather have a huge multitude of possible candidates, and sometimes we need to **transform** between these. How to perform these transformations and still preserve the physics and numerical stability, depend on our chosen **gauge**, and is a major part later in this thesis.

We'll now take a series of detours to lay the foundation of what we need in order to fully appreciate the field of cosmology. Note that we assume the reader to be familiar with Special Relativity.

2.4 General Relativity

General relativity (GR) is Einstein's theory of space, time and gravitation [4], and in short terms tells us that gravity is a manifestation of the curvature of spacetime itself, unlike other fields defined on the spacetime (electromagnetic fields etc). It can be said that GR is a particular example of classical field theory, so let us take a quick detour by looking at classical fields defined on a flat spacetime.

2.4.1 Classical Field Theory

When Newton's laws break down, i.e. when we move on to more complex systems where Newton's second law becomes too unwieldy, we can turn to Hamilton's Principle, which is formulated in terms of an action integral,

$$S = \int_{t_1}^{t_2} L(q_i(t), \dot{q}_i(t))\, dt, \tag{2.2}$$

where q_i is a generalized coordinate and L is the Lagrangian of the system and is defined as $L = T - V$, where T is the kinetic energy, and V is the potential energy.

The principle states that the path $q_i(t)$ between the points at t_1 and t_2, which describe the evolution of the system [8], is characterized by the action being stationary under small variations in the path $q_i(t) \to q_i(t) + \delta q_i(t)$, with $\delta q_i(t_1) = \delta q_i(t_2) = 0$. This condition can be written as

$$\delta S = \int_{t_1}^{t_2} \delta L\, dt = 0. \tag{2.3}$$

Note that this is also often referred to as the "principle of least action".

This requires a variation of the Lagrangian itself, and gives rise to the so-called Euler-Lagrange (EL) equations,

$$\begin{aligned} \delta S = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q_i} \delta q_i - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \delta q_i \right] dt = 0 \\ \Rightarrow \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0. \end{aligned} \tag{2.4}$$

Field theory is very similar, the coordinate $q(t)$ is replaced by a set of spacetime-dependent fields $\Phi^i(x^\mu)$, and S is now a functional[6] of these fields. The Lagrangian is expressed as an integral over space of a Lagrangian density $\mathcal{L}$ (now a function of the field Φ^i and their spacetime derivatives $\partial_\mu \Phi^i$),

$$L = \int d^3x\, \mathcal{L}(\Phi^i, \partial_\mu \Phi^i) \;\Rightarrow S = \int d^4x\, \mathcal{L} \tag{2.5}$$

[6] A functional is a function of an infinite number of variables.

Similarly to earlier, we can find new Euler-Lagrange equations keeping the same form as earlier,

$$\frac{\partial \mathcal{L}}{\partial \Phi^i} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi^i)} \right) = 0. \tag{2.6}$$

For deeper discussion of this I refer the reader to [4] as a great source.

2.4.2 The Metric and Line Element

The metric is a symmetric tensor that plays an important role in all of GR and cosmology. The metric, $g_{\mu\nu}$, has to be a symmetric tensor that is non-degenerate (the determinant $g = |g_{\mu\nu}| \neq 0$), so that the inverse metric $g^{\mu\nu}$ is defined as,

$$g^{\mu\nu} g_{\nu\sigma} = \delta^\mu_\sigma, \tag{2.7}$$

where the symmetry of $g_{\mu\nu}$ implies symmetry in $g^{\mu\nu}$. We can use this to raise and lower indices, just as in Special Relativity [4, 5].

The metric $g_{\mu\nu}$ has numerous special abilities worth noting. In the words of Carroll [4], it supplies a notion of "past" and "future", it allows the computation of path length and proper time, it determines the "shortest distance" between two points and therefore the motion of "test particles", it replaces the the Newtonian gravitational field Φ, and it defines the speed of light.

Next we define the line element,

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu, \tag{2.8}$$

where dx^μ is an infinitesimal displacement in the direction of x^μ. The line element is used to present what kind of universe we are looking at, and is supplied instead of the metric itself throughout the literature.

2.4.3 The Tools of GR

In order to perform calculations within GR, there are several tools we need to know how to use. First up is the **Christoffel** connection Γ, where the Christoffel symbols are defined by

$$\Gamma^\mu_{\alpha\beta} = \frac{g^{\mu\nu}}{2} \left[g_{\alpha\nu,\beta} + g_{\nu\beta,\alpha} - g_{\alpha\beta,\nu} \right]. \tag{2.9}$$

This is one of the biggest building blocks of GR, and will be used every time we do calculations in GR.

Next up, using the Christoffel symbols, we define the **Ricci tensor** $R_{\mu\nu}$ as

$$R_{\mu\nu} = \Gamma^\alpha_{\mu\nu,\alpha} - \Gamma^\alpha_{\mu\alpha,\nu} + \Gamma^\alpha_{\alpha\beta}\Gamma^\beta_{\mu\nu} - \Gamma^\alpha_{\beta\nu}\Gamma^\beta_{\mu\alpha}. \tag{2.10}$$

We can then continue by taking the trace of equation (2.10) to find the **Ricci scalar**,

$$R = R^\mu_\mu = g^{\mu\nu} R_{\mu\nu}, \tag{2.11}$$

which is the final piece we need to construct the **Einstein tensor** $G_{\mu\nu}$,

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}. \tag{2.12}$$

The Einstein tensor is the left hand side of **Einstein's equation**,

$$G_{\mu\nu} = \kappa^2 T_{\mu\nu}, \tag{2.13}$$

where $T_{\mu\nu}$ is the stress-energy tensor and $\kappa^2 = 8\pi G = m_{Pl}^{-2}$.

2.4.4 The Stress-Energy Tensor

The stress-energy tensor is a tensor used to express the matter content of the Universe, if we assume the Universe to be composed of various fluids, both effective fluids (photons, neutrinos) and actual fluids (baryons, cold dark matter). For a general fluid the stress-energy tensor is given by

$$T_{\mu\nu} = (\rho + p) u_\mu u_\nu + p g_{\mu\nu} + 2 q_{(\mu} u_{\nu)} + \pi_{\mu\nu}, \tag{2.14}$$

where ρ and p are the energy and momentum density of the fluid, q is the heat flow and $\pi_{\mu\nu}$ is the anisotropic stress[7], and u_μ is the four-velocity of the fluid defined as

$$u^\mu = \frac{dx^\mu}{\sqrt{-ds^2}}, \tag{2.15}$$

which has the property $u^\mu u_\mu = -1$, with the heat-flow vector q_μ and anisotropic stress tensor $\pi_{\mu\nu}$ satisfying $u^\mu q_\mu = u^\mu \pi_{\mu\nu} = g^{\mu\nu} \pi_{\mu\nu} = 0$. We will return to further discussion of the stress-energy tensor once we have more of the formalism pinned down.

2.4.5 Lagrangian Formalism of GR

This is the point where §2.4.1 comes into play. GR can, as mentioned, be seen as a particular example of a classical field, and we now show that we can get to equation (2.13) from a field-theoretical viewpoint. We start out with an action consisting of the Einstein-Hilbert action and the action for matter and energy [5] of the form

$$S = S_{EH} + S_M = \frac{1}{2\kappa^2} \int (R - 2\Lambda) \sqrt{-g}\; d^4x + \int \mathcal{L}_M \sqrt{-g}\; d^4x, \tag{2.16}$$

where this R is the Ricci scalar, Λ is the cosmological constant and $\mathcal{L}_M$ is the Lagrangian density for matter and energy. We're going to use the principle of least action to get to the Einstein equations. First, vary equation (2.16) with respect to the inverse metric, with $\delta g_{\mu\nu} = -g_{\mu\rho} g_{\nu\sigma} \delta g^{\rho\sigma}$,

$$\delta S = \delta S_{EH} + \delta S_M = 0. \tag{2.17}$$

[7] We typically neglect the heat flow and the anisotropic stress, reintroducing them in Chapter 6.

We will find these terms separately, first for the Einstein-Hilbert part δS_{EH} and then for the matter part δS_M. We then get

$$\delta S_{EH} = \frac{1}{2\kappa^2}\int \left[\sqrt{-g}\delta R + (R-2\Lambda)\delta\sqrt{-g}\right] d^4x. \tag{2.18}$$

We continue by finding δR, where we use the definition of the Ricci scalar, equation (2.11), so that

$$\delta R = R_{\mu\nu}\delta g^{\mu\nu} + g^{\mu\nu}\delta R_{\mu\nu}, \tag{2.19}$$

where the first term is already proportional to $\delta g^{\mu\nu}$ and is therefore done, while the second term will disappear when integrated thanks to Stokes' Theorem or Gauss' integral theorem [5],

$$\int d^4x g^{\mu\nu}\sqrt{-g}\delta R_{\mu\nu} = 0.$$

We then look at the term $\delta\sqrt{-g}$. To get anywhere we must use some general properties for any square matrix M with non-vanishing determinant $\det(M)$,

$$\ln\det(M) = \mathrm{Tr}(\ln M) \Rightarrow \frac{1}{\det(M)}\delta\det(M) = \mathrm{Tr}(M^{-1}\delta M).$$

We let $M = g_{\mu\nu}$ and $\det(M) = g$ so that

$$\delta\sqrt{-g} = -\frac{1}{2\sqrt{g}}\delta g = -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta g^{\mu\nu}. \tag{2.20}$$

This then gives us,

$$\delta S_{EH} = \frac{1}{2\kappa^2}\int \sqrt{-g}d^4x\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}(R-2\Lambda)\right]\delta g^{\mu\nu}. \tag{2.21}$$

Similarly we find

$$\begin{aligned}\delta S_M &= \int d^4x\left[\mathcal{L}\delta\sqrt{-g} + \sqrt{-g}\delta\mathcal{L}\right] = \int d^4x\sqrt{-g}\left[\frac{\delta\mathcal{L}}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}\mathcal{L}\right]\delta g^{\mu\nu}\\ &= \int d^4x\sqrt{-g}\left[-\frac{1}{2}T_{\mu\nu}\right]\delta g^{\mu\nu},\end{aligned} \tag{2.22}$$

where we defined the stress-energy tensor as $T_{\mu\nu} = -2\left[\frac{\delta\mathcal{L}}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}\mathcal{L}\right]$. We then use the principle of least action to get

$$\delta S = \delta S_{EH} + \delta S_M = 0 \Rightarrow \delta S_{EH} = -\delta S_M,$$

so that

$$\begin{aligned}\frac{1}{2\kappa^2}\left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}(R-2\Lambda)\right) &= \frac{1}{2}T_{\mu\nu}\\ \Rightarrow \boxed{R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + g_{\mu\nu}\Lambda = \kappa^2 T_{\mu\nu}}&.\end{aligned} \tag{2.23}$$

We see that equation (2.23) is equal to equation (2.13) when we remove the cosmological constant. For the majority of this thesis we will be working with $\Lambda = 0$.

2.5 Modifying General Relativity

Now that we know how standard gravity theory works, we'll take a look at how we can modify it, which we want to do in order to explain observed effects that are not explained by standard GR. In its simplest form, Einstein's equation is,

$$G_{\mu\nu} = \kappa^2 T_{\mu\nu} \tag{2.24}$$

and ,as is obvious, modifications have to be made either to the right hand side or the left hand side. Changing the right hand side,

$$G_{\mu\nu} = \kappa^2 \left(T_{\mu\nu} + T_{\mu\nu}^{DE}\right), \tag{2.25}$$

is the equivalent of adding some unknown matter to our theory (mostly dark energy and dark matter, as used above), which will correct the results the theory give us to coincide with the observed results. Alternatively, we can modify the left hand side,

$$G_{\mu\nu} + G_{\mu\nu}^{MOD} = \kappa^2 T_{\mu\nu}, \tag{2.26}$$

which is the same as reevaluating our understanding of the fabric of space-time, without adding mysterious unknown particle-species or energies to the Universe. This latter modification is the one we will be focusing on in this thesis.

2.5.1 Modified Gravity

When modifying gravity, the Einstein-Hilbert Lagrangian density $\mathcal{L}_{\mathrm{EH}} = R$ is typically replaced by a much more general function including terms of higher order in derivatives of the metric (R^2, $R_{\mu\nu}R^{\mu\nu}$, $R_{\alpha\beta\mu\nu}R^{\alpha\beta\mu\nu}\ldots$) and couplings to new dynamical degrees of freedom. This kind of extended gravity has seen an increase in applications to cosmology; see [9] and its references for an overview and further details on these models and their applications to cosmology.

Lately the literature has focused on using modified gravity to model dark energy without the need to introduce exotic particles. One of the most employed models in this context is $f(R)$ gravity (see [10] for a deeper review than this thesis will give), where the Einstein-Hilbert Lagrangian density is replaced with an arbitrary function of the Ricci scalar, $\mathcal{L} = f(R)$. This representation of an extended gravity model is known as the "Jordan frame".

With this formulation the action can be transformed to a variety of different forms. One of the most frequent of these transformations shows us that $f(R)$ gravity can be considered a class of Brans-Dicke theories; see §3.1.1. We can also transform into the so-called "Einstein frame", which can be viewed as simply an alternative reference frame where the action is manipulated to isolate a Ricci scalar of a the metric. The field equations are otherwise those of standard general relativity.

As the main focus of this thesis is on $f(R)$ models and their properties, we'll return to $f(R)$ in Chapter 3.

2.5.2 Transformation Between Frames

We just mentioned two different frames, the Jordan and Einstein frames, and that we can transform between them. But why would we want to do that, how, and why is there so much controversy around it?

In the Jordan frame the action is varied directly with respect to the metric, and the field equations are immediately fourth order. In the Einstein frame, as in standard GR, the theory is second order, a significant simplification. The transformation, which is conformal so that the causal structure of spacetime is unaffected by the transformation, is

$$g_{\mu\nu} \to \tilde{g}_{\mu\nu} = \Omega^2 g_{\mu\nu} \Rightarrow \tilde{g}^{\mu\nu} = \Omega^{-2} g^{\mu\nu}, \quad \tilde{g} = \Omega^8 g, \tag{2.27}$$

where Ω is the conformal transformation factor [10] and a tilde represent quantities in the Einstein frame. With $\ln\Omega = \omega$, the Christoffel symbols, covariant derivatives of a scalar and a covector, the Ricci tensor, Ricci scalar, stress-energy tensor, stress-energy conservation transform [11, 12, 13, 9] as,

$$\tilde{\Gamma}^{\lambda}_{\mu\nu} = \Gamma^{\lambda}_{\mu\nu} + \left(2\delta^{\lambda}_{(\mu}\nabla_{\nu)}\omega - g_{\mu\nu}\nabla^{\lambda}\omega\right), \quad \tilde{\nabla}_\mu\phi = \nabla_\mu\phi \tag{2.28}$$

$$\tilde{\nabla}_\mu v_\nu = \nabla_\mu v_\nu - \left(2\delta^{\lambda}_{(\mu}\nabla_{\nu)}\omega - g_{\mu\nu}\nabla^{\lambda}\omega\right) v_\lambda, \quad \tilde{T}^{(M)}_{\mu\nu} = \Omega^{-2} T^{(M)}_{\mu\nu}, \tag{2.29}$$

$$\tilde{\rho}_{\mu\nu} = R_{\mu\nu} - 2\nabla_\mu\nabla_\nu\omega - g_{\mu\nu}\nabla^\alpha\nabla_\alpha\omega + 2\nabla_\mu\omega\nabla_\nu\omega - 2g_{\mu\nu}\nabla^\alpha\omega\nabla_\alpha\omega \tag{2.30}$$

$$\tilde{\rho} = \Omega^{-2}\left(R - 6\nabla^\mu\nabla_\mu\omega - 6\nabla^\mu\omega\nabla_\mu\omega\right), \tag{2.31}$$

with the matter continuity in the Einstein frame being

$$\tilde{\nabla}_\mu\tilde{T}^{\mu\nu}_{(M)} = -\tilde{T}_{(M)}\tilde{\nabla}^\nu\omega. \tag{2.32}$$

Aspects of the transformation have been controversial for some time (see for example [13, 14, 15, 9]; I present further references in §3.3). The discussion has centred upon the nature of the equivalence of quantities in the two frames, and authors can be separated [13, 9] into two camps: those who feel the equivalence is "physical" and observables can be calculated in either frame, and those who feel the equivalence is mathematical in nature and that observables should be calculated in a chosen "physical frame". We briefly discuss this issue in §3.3.

However, our work on this controversy has revealed an as yet unappreciated issue. Perturbed systems in relativity exhibit the gauge issue, the issue of choosing the best way to map between the fictitious background spacetime and the physical perturbed spacetime. In cosmology, gauge freedoms allow one to eliminate four of the ten degrees of freedom in the metric perturbation (two scalar and two vector), which specifies the "slicing and threading" we have chosen for our foliation.[8]

It turns out that the transformation between the Einstein and the Jordan frames tangles this choice of slicing and threading. We consider the impact of this and how one

[8]By slicing and threading the foliation we talk about the way we choose the coordinates of the metric. More on this later.

can resolve the resulting gauge ambiguities, by illustrating with a simple $f(R)$ model in a vacuum FLRW spacetime, but it should be emphasized that this issue will in principle occur in any perturbed spacetime and a wide range of extended theories of gravity, in Chapter 5.

2.6 Modern Cosmology

With the mathematical groundwork laid down before us, we can start taking a look at the field of modern cosmology.

2.6.1 The Friedmann-Lemaître-Robertson-Walker Metric

The FLRW[9] metric is the most used metric in the modern literature. It arises as an exact solution of Einstein's field equations (2.13) for a homogeneous and isotropic expanding/contracting universe,

$$ds^2 = a(\eta)^2 \left(-d\eta^2 + \frac{dr}{1-kr^2} + r^2 d\theta^2 + r^2 \sin\theta d\phi^2 \right), \tag{2.33}$$

where θ, ϕ and r are polar coordinates in the radial form, while k is the curvature parameter. The curvature parameter is usually chosen to be either

- $k = 1$, representing a closed universe without boundaries that might collapse the Universe down to a Big Crunch.
- $k = -1$, representing an open, ever-expanding universe.
- $k = 0$, representing a flat universe.

Throughout this thesis we will be working in a flat universe, and the equations therefore simplify significantly.

2.6.2 Redshift as a Measure of Time

From the FLRW metric (2.33) we can easily derive a relation [7] between the scale factor and wavelength such that

$$\frac{\lambda_0}{\lambda_e} = \frac{a(\eta_0)}{a(\eta_e)},$$

where λ_0 and λ_e is the wavelength observed today and at an emitted time η_e respectively. We can therefore measure how much the observed light has been stretched during its

[9] Since the dynamics of the FLRW model were proposed by Friedmann and Lemaître, the latter two names are often omitted by cosmologists outside of the USA. However, cosmologists in USA often only refer to the latter two names, a "Robertson-Walker" model. The full four-name title is the most democratic, and is therefore the one I use in this thesis.

travel to us to find the size of the scale factor, and hence the size of the Universe, at time of emission compared to today. From this one defines the redshift z as

$$1 + z = \frac{a_0}{a_e}. \tag{2.34}$$

As is obvious, light emitted today have a redshift of $z = 0$, while in the very early universe it would be $z \approx \infty$.

2.6.3 The Friedmann Equations

The Friedmann equations are some of the most used equations in all of cosmology, as they tell us how the scale factor a evolves with time, and can be used to simulate different universe models. To get the Friedmann equations, we start with the flat Friedmann-Robertson-Walker (FLRW) metric in Cartesian coordinates,

$$ds^2 = a^2(\eta)(-d\eta^2 + \delta_{ij}dx^i dx). \tag{2.35}$$

We then use the mathematical groundwork of GR we showcased in §2.4.3 to find the Christoffel symbols,

$$\begin{aligned} \Gamma^0_{00} &= \mathcal{H}, \\ \Gamma^0_{ij} &= \mathcal{H}\delta_{ij}, \\ \Gamma^i_{0j} &= \Gamma^0_{ij}, \end{aligned} \tag{2.36}$$

where we have introduced the conformal Hubble parameter as $\mathcal{H} = \frac{\dot{a}}{a}$. We then find the Ricci tensor and finally the Ricci scalar itself,

$$\left.\begin{aligned} R_{00} &= -3\left(\frac{\ddot{a}}{a} - \mathcal{H}^2\right) \\ R_{ij} &= \left(\frac{\ddot{a}}{a} + \mathcal{H}^2\right)\delta_{ij} \end{aligned}\right\} \Rightarrow R = \frac{6}{a^2}\frac{\ddot{a}}{a}. \tag{2.37}$$

We implement these components into the Einstein equation (2.23), and first look at the time-time component to get the first Friedmann equation,

$$\mathcal{H}^2 = \frac{\kappa^2}{3}\rho a^2, \tag{2.38}$$

where the right hand side come from analyzing the stress-energy tensor for this metric,

$$T_{00} = (\rho + p)u_0 u_0 + p g_{00} = (\rho + p)a^2 - pa^2 = \rho a^2. \tag{2.39}$$

Likewise, looking at the spatial-component give us the second Friedmann equation[10],

$$\frac{\ddot{a}}{a} = \frac{\kappa^2}{6}(\rho - 3p)a^2. \tag{2.40}$$

[10]Sometimes erroneously referred to as the Raychaudhuri equation.

Combining these two equations, we get an expression for the evolution of the density,

$$\dot{\rho} = -3\mathcal{H}(\rho + p). \tag{2.41}$$

At this point we should bring up the equation of state, which is a simple relation between the pressure p and the density ρ, given as,

$$p = w\rho, \tag{2.42}$$

where the equation of state parameter w is a free parameter that is dependant on the gas we discuss. The speed of sound is given as[11],

$$c_s^2 = \frac{\partial p}{\partial \rho} = w + \frac{\partial w}{\partial \rho}\rho. \tag{2.43}$$

2.6.4 Different Universe Models

Selecting different values of w is the most common way for cosmologists to describe different kinds of universes, or simply different epochs of our universe. From equation (2.41) and equation (2.42) we can find an expression for how the energy density evolves with the scale factor of the Universe. We start by rewriting equation (2.41),

$$\dot{\rho} = -3\mathcal{H}(1 + w)\rho, \tag{2.44}$$

which can be further rewritten as a differential equation

$$\frac{d\rho}{\rho} = -3(1 + w)\frac{da}{a}. \tag{2.45}$$

Integrating this from a scale factor a until the scale factor today a_0 we get,

$$\rho = \rho_0 \left(\frac{a_0}{a}\right)^{3(1+w)}, \tag{2.46}$$

where ρ_0 is the present day value of the energy density. Similarly, we can find an expression for the scale factor of the universe as a function of conformal time η. In order to do this we introduce the density parameter Ω, which is defined as the ratio between the density of a fluid and the critical density ρ_c,

$$\rho_c = \frac{3\mathcal{H}_0^2}{\kappa^2} \Rightarrow \Omega_0 = \frac{\rho_0}{\rho_{c0}} = \frac{\kappa^2 \rho}{3\mathcal{H}_0^2}. \tag{2.47}$$

For a flat universe, $\Omega_0 = 1$, and $\rho_0 = \rho_c$. With this, we can insert equation (2.46) into our first Friedmann equation (2.38) (while tweaking a bit to emphasize the critical density) to find

$$\left(\frac{\dot{a}}{a}\right)^2 = a^2\mathcal{H}_0^2 \frac{\kappa^2}{3\mathcal{H}_0^2}\rho_0 \left(\frac{a_0}{a}\right)^{3(1+w)} = a^2\mathcal{H}_0^2 \left(\frac{a_0}{a}\right)^{3(1+w)},$$

[11]This expression is not entirely valid; in general we have from thermodynamics and statistical physics that $\delta p = \frac{\partial p}{\partial \rho}|_S \delta\rho + \frac{\partial p}{\partial S}|_\rho \delta S$. However we assume that the fluid is barotropic and irrotational so that we can assume $\frac{\partial p}{\partial S} = 0$.

which we turn into a differential equation integrated from a distant time η to the present time of η_0,

$$a_0^{3(1+w)/2}\int_{a_0}^{a} a'^{\frac{3w}{2}-\frac{1}{2}}da' = \mathcal{H}_0\int_{\eta_0}^{\eta} d\eta'.$$

This is easily solved to give us

$$\frac{2}{3(1+w)a_0}\left[\left(\frac{a}{a_0}\right)^{(3w+1)/2} - 1\right] = \mathcal{H}_0(\eta-\eta_0), \tag{2.48}$$

which is a closed solution. However we can improve it by choosing the time where the scale factor vanished to be at $\eta = 0$. Imposing $a = 0$ at $\eta = 0$ we find

$$\frac{2}{3(1+w)a_0} = \mathcal{H}_0\eta_0,$$

which when inserted into equation (2.48) gives us

$$\mathcal{H}_0\eta_0\left(\frac{a}{a_0}\right)^{(3w+1)/2} = \mathcal{H}_0\eta \Rightarrow a(\eta) = a_0\left(\frac{\eta}{\eta_0}\right)^{\frac{2}{3w+1}}. \tag{2.49}$$

From this we can also find how the Hubble parameter scales,

$$\mathcal{H} = \frac{2}{(3w+1)\eta}. \tag{2.50}$$

Dust filled universes

A dust filled universe is a universe filled with non-relativistic matter, such as most of the visible matter of our universe (i.e. the matter in galaxies). As mentioned, cosmologists use the equation of state parameter w to differentiate between universe models, so what would w be for a dust-filled universe? From thermodynamics we know that the pressure for a gas of N particles with mass m, temperature T in a low density volume V is

$$p = \frac{Nk_BT}{V},$$

where k_B is the Boltzmann's constant. Introducing the mass density of such a gas as $\rho = mN/V$, and keeping in mind that the mean square velocity of an ideal gas is $m\langle v^2\rangle = 3k_BT$, we can rewrite the pressure as,

$$p = \frac{\langle v^2\rangle}{3}\rho \Rightarrow w = \frac{\langle v^2\rangle}{3}, \tag{2.51}$$

giving us the equation of state parameter for a dust filled universe. However as we imposed non-relativistic matter, we know that $v \ll 1$ and it is thus justified to approximate $w \approx 0$ for a dust-filled universe. This also tells us that such an universe is pressure-less.

By now inserting $w = 0$ into equation (2.49) we find that for a dust filled universe the scale factor evolves as

$$a(\eta) = a_0 \left(\frac{\eta}{\eta_0}\right)^2, \tag{2.52}$$

while from equation (2.50) we find that the Hubble parameter evolves as

$$\mathcal{H} = \frac{2}{\eta}. \tag{2.53}$$

This universe model is called a Einstein-de Sitter model, and was a favourite among cosmologists for a long time [7].

Radiation filled universes

A radiation filled universe is, on the other hand, a universe filled with relativistic, massless particles, such as photons and neutrinos[12]. Finding the equation of state parameter is much easier in this case, as we already know that for a gas of photons, the pressure is

$$p = \frac{1}{3}\rho, \tag{2.54}$$

and we immediately see that $w = \frac{1}{3}$ for a radiation dominated universe. This model is very good at representing the Universe at earlier times, when the temperature was sufficiently high that it was dominated by radiation.

By now inserting $w = 1/3$ into equation (2.49) and equation (2.50) we find that for a radiation universe the scale factor and Hubble parameter are

$$a(\eta) = a_0 \left(\frac{\eta}{\eta_0}\right) \text{ and } \mathcal{H} = \frac{1}{\eta}. \tag{2.55}$$

Universe with a cosmological constant

When Einstein first applied his theory of GR to the Universe as a whole, he soon discovered that his solution gave a collapsing Universe. As such a thing was unthinkable to the physicists at the time, he decided to modify his equations so that the result would be a static, homogeneous and isotropic universe, by adding a constant, known as the cosmological constant. If we keep the cosmological constant in our Einstein field equation (2.13) to re-derive the first Friedmann equation (2.38) we get

$$\mathcal{H}^2 = \frac{\kappa^2}{3}\rho a^2 + \frac{\Lambda}{3}a^2. \tag{2.56}$$

[12]Neutrinos have been shown to actually have mass, however we can still treat them as massless particles simply because their mass is so very small that the approximation is generally valid.

If we now wish to view the cosmological density as a contribution to the energy density of the Universe, we can insert ρ_Λ into the first Friedmann equation (2.38) and quickly find that

$$\rho_\Lambda = \frac{\Lambda}{\kappa^2}. \tag{2.57}$$

By also finding the second Friedmann equation with a cosmological constant,

$$\frac{\ddot{a}}{a} = \frac{\kappa^2}{6}a^2\rho + \frac{2}{3}\Lambda a^2, \tag{2.58}$$

and comparing this to equation (2.40) with ρ_Λ and p_Λ inserted we see that

$$\frac{\kappa^2}{6}(\rho + \rho_\Lambda - 3p_\Lambda)a^2 = \frac{\kappa^2}{6}a^2\rho + \frac{2}{3}\Lambda a^2,$$

which gives us

$$p_\Lambda = -\frac{\Lambda}{\kappa^2} = -\rho_\Lambda, \tag{2.59}$$

revealing to us that a universe with a cosmological constant can be described by an equation of state parameter $w = -1$. For a positive cosmological constant this tells us that we have a negative pressure, which can be interpreted as repulsive gravity! This kind of universe is called a de Sitter universe, and is characterized by the fact that it has an exponential expansion. De Sitter universes will be of much use as we get to inflation.

In order to find the evolution of the scale factor and Hubble rate in a conformal time de Sitter universe, we first return to cosmic time, as the derivation otherwise gets highly convoluted. The scale factor evolves in coordinate time de Sitter space as [7]

$$a(t) = a_0 e^{H_0(t-t_0)}, \tag{2.60}$$

with

$$H_0 = \sqrt{\frac{\Lambda}{3}}. \tag{2.61}$$

Inserting this scale factor into equation (1.1) we get

$$\eta = \int_0^t e^{-H_0 t} dt = -\frac{1}{H_0}\left(e^{-H_0 t} - 1\right) \tag{2.62}$$

$$\Rightarrow e^{H_0 t} = (1 - H_0\eta)^{-1}. \tag{2.63}$$

This gives us

$$a(\eta) = a_0 (1 - H_0\eta)^{-1} \tag{2.64}$$

and

$$\mathcal{H} = \frac{H_0}{1 - H_0\eta}. \tag{2.65}$$

Mixed universes

As will come as no surprise, our Universe cannot be explained with just one of the above three models; we have to mix them all together. The general consensus today is that it started out in a radiation dominated state, then phased over to be matter (dust) dominated, and is today at the crossing between being matter and "dark energy" dominated. Therefore it is of interest to calculate exactly when this transition from radiation to matter domination transpired. By using equation (2.46) we can see how radiation and matter density scale with the scale factor:

$$\rho_r = \rho_{r0}\left(\frac{a_0}{a}\right)^4 = p_{c0}\Omega_{r0}\left(\frac{a_0}{a}\right)^4,$$
$$\rho_m = \rho_{m0}\left(\frac{a_0}{a}\right)^3 = p_{c0}\Omega_{m0}\left(\frac{a_0}{a}\right)^3.$$

As goes without saying, to find the moment of equality, we set $\rho_r = \rho_m$ and define the scale factor at which this was true to be $a = a_{eq}$ to find

$$a_{eq} = a_0\frac{\Omega_{r0}}{\Omega_{m0}}. \tag{2.66}$$

With today's observed values this corresponds to a redshift of $z = 3570$.

The current favoured universe

We're ending this section with a brief mention of what is the preferred model according to astronomers today, and that is the ΛCDM model, which essentially is a universe dominated by dark energy represented by a positive cosmological constant, with dust mostly in the form of cold dark matter (CDM). This model is sometimes referred to as the concordance model. For more on this model I refer the reader to [7, 5] or any other modern cosmology textbook.

2.7 Inflation

Having so far had a brief overview of the history of the Universe, looked at the mathematical background and now seen how the different Universe models are built up in modern cosmology, it is time to delve deeper into the topic of inflation. Inflation was briefly mentioned earlier in §2.2; however we did not discuss how the idea of inflation was first introduced. It turns out that standard Big Bang cosmology is riddled with problems, and inflation might just be the way to solve them.

2.7.1 Problems with the Big Bang Model

Of the various problems in the Big Bang model, we'll only look at the three biggest problems; for anything else I refer the reader to [6, 7].

Flatness problem

We have throughout this thesis been working in a flat $k = 0$ universe, simply since this seems to be the way the Universe is today; however one of the problems of the Big Bang model can be shown by keeping the k in our equations: the curvature of the Universe increase with time [6, 7]. In fact, it can be shown that the deviation from flatness evolves as[13],

$$\Omega(t) - 1 \propto t^{2/3},$$

telling us that if we today have $\Omega - 1 = 0.02$, then at the Planck time t_{Pl} it would have to be 10^{-60} times smaller than today. Such an extreme adjustment can not be explained within the old Big Bang model, and something new is needed to fix this.

Horizon problem

This problem arise from the fact that the Universe has a finite age, and has thus only had a finite time in which to send photons, which can only have travelled a finite distance. One of the most important aspects of the CMB, which we discuss further in §2.8.1, is that light measured from all directions in the sky register at the same temperature of 2.7 K. If parts of the Universe have the same temperature, it stands to reason that they have at one time been interacting, in order to reach thermal equilibrium. However, light that we observe from one end of the Universe has been travelling towards us since decoupling, as has also the light we observe from the other end of the Universe. There has therefore not been enough time for the regions the photons originate from to have interacted and established thermal equilibrium, and they should not be at the same temperature. Again, we need something new to fix this.

Monopole problem

This problem only comes up with attempts to combine the Big Bang model with modern particle physics, most notably particles needed for the Grand Unified Theories to be valid [16], such as the monopole. Such monopoles are supposed to be extremely massive - so massive, in fact, that they would come to dominate the Universe and end the radiation dominated era of the Universe much earlier than we know it ended. As particle physics has evolved, even more problematic particles have been introduced, with the same problems as the monopoles, such as gravitinos and so on.

[13] We'll return to cosmic time as all the literature is given in cosmic time, and this is not an important enough equation for us to take the time to re-derive it in conformal time.

2.7.2 Cue Inflation

In 1981 Alan Guth proposed inflation[14] as a way to solve all of these problems, and more not discussed here. The core of inflation is that it is defined as a period of the Universe when the scale factor was accelerating, so let us introduce the so-called deceleration parameter[15] in conformal time,

$$q = -\frac{\dot{\mathcal{H}}}{\mathcal{H}^2} = 1 - \frac{a\ddot{a}}{\dot{a}^2}. \tag{2.67}$$

In order to produce an accelerating universe, q has to be negative, which is only achieved if

$$\frac{a\ddot{a}}{\dot{a}^2} > 1 \Rightarrow \frac{\ddot{a}}{a} > \mathcal{H}^2;$$

inserting our expressions for $\frac{\ddot{a}}{a}$ and $\mathcal{H}^2$ gives

$$\frac{\kappa^2}{6}(\rho - 3p)a^2 > \frac{\kappa^2}{3}\rho a^2,$$

resulting in

$$p < -\frac{\rho}{3}. \tag{2.68}$$

So in order to have an accelerating universe, we need a negative pressure!

If we remember back to the previous section, we've already encountered negative pressure in the de Sitter universe. This tells us that the inflation era operates just like a de Sitter universe would if we set $w = -1$, and as we did when we discussed the de Sitter universe earlier, we return to cosmic time for easier calculations. With the expression for a de Sitter scale factor (2.60), we see that

$$\Omega(t) - 1 \propto \frac{1}{a^2H^2} = e^{-2H_0t}$$

is now a decreasing function of time. This means, as long as the Universe is expanding at an exponential rate, any deviations from flat space will be killed off by the expansion! To clarify with the words of Elgarøy [7], "if a region of the universe was not spatially flat to begin with, the enormous expansion rate would blow it up and make its radius of curvature infinitesimally small". As easily as that the flatness problem is solved.

[14] Although Alexei Starobinsky had already developed the first realistic inflation model in 1979, he failed to relate its relevance to modern cosmological problems, such as those just discussed. As well as this, the political climate of the world during the Cold War ensured that most cosmologists outside of the USSR were unaware of Starobinsky's work until many years later. On top of all of this Starobinsky's model said little about how the inflation process could start.

[15] The name is a relic from the time when scientists believed the Universe to be decelerating, not suspecting it could be a negative quantity. The traditional cosmic time variant is $q = a''a/a'^2$, where a prime denotes derivative with respect to cosmic time.

The horizon problem is also easily fixed by the fact that a small region of the Universe that was small enough to form thermal equilibrium, expands by inflation to a size larger than our observable universe. So photons we observe from opposite sides of the Universe today have actually been causally connected in the distant past, and no problem remains. The monopole/relic problem however, is explained simply through the fact that these massive particles have been diluted by the extreme expansion. They are still around, but with the expansion we can easily explain why we do not observe them. But how much did the Universe actually expand?

From [7, 17] it is shown that for inflation starting at time t_i and ending at t_f,

$$\frac{a(t_f)}{a(t_i)} = e^N, \tag{2.69}$$

where N is the number of "e-foldings", i.e. the number of times the Universe has expanded by a factor e, given by

$$N = H_i(t_f - t_i). \tag{2.70}$$

It is generally assumed that inflation lasted for $N \sim 60$ e-foldings, more than sufficient enough to solve all the problems we've discussed. In this thesis we will typically take $N = 55$.

2.7.3 Driving Force of Inflation

Having now seen why we need inflation, and what it is, we need to figure out how inflation starts, maintains for ~ 60 e-foldings, and ends in a timely manner. However these aspects of inflation is still not well understood, the most common idea is that inflation is driven by one or more scalar fields.

By analogy with vector fields such as the electromagnetic fields, which we assume the reader to be familiar with, a scalar field is a way to associate a real number with a point in space at a given time, such as the temperature of the Earth's atmosphere.[16] The most important thing we need to know about a scalar field is that it has a kinetic and potential energy, which in turn tell us that it has an energy density and a pressure. Let us now focus on a homogeneous scalar field ϕ, homogeneous meaning it only depends on time, where the energy density and pressure in an FLRW universe are given b,

$$\rho_\phi = \frac{1}{2a^2}\dot{\phi}^2 + V(\phi) \tag{2.71}$$

and

$$p_\phi = \frac{1}{2a^2}\dot{\phi}^2 - V(\phi), \tag{2.72}$$

[16] Note however, that unlike the temperature the scalar field is a physical quantity.

where $V(\phi)$ is the potential energy of the field. We can also note that imposing that the field varies slowly in time, so that

$$\dot{\phi}^2 \ll 2a^2V(\phi), \tag{2.73}$$

will give us an equation of state

$$p_\phi = -\rho_\phi,$$

exactly as a cosmological constant would. This final aspect is what gives us the idea of using scalar fields to drive inflation. From quantum field theory [16] we have the Klein-Gordon equation

$$\Box\phi - V_{,\phi} = 0, \tag{2.74}$$

which when using the FLRW metric give the evolution of the scalar field as

$$\ddot{\phi} + 2\mathcal{H}\dot{\phi} + a^2V_{,\phi} = 0. \tag{2.75}$$

Upon closer inspection, we recognize this equation as that of a ball rolling down a hill, or more generally, as the equation of motion for a particle moving along the x-axis in a potential well $V(x)$. With this analogy, ϕ is the coordinate of the particle and $2\mathcal{H}\dot{\phi}$ is the frictional force supplied by the expansion of the Universe. Similarly, we would expect to find a terminal "velocity" of the field as well, the point at which $\ddot{\phi} = 0$:

$$\dot{\phi} = -\frac{a^2}{2\mathcal{H}}V_{,\phi}. \tag{2.76}$$

If we now insert this "velocity" into our constraint for the scalar field to behave like a cosmological constant equation (2.73), in order to get the constraint in terms of more familiar quantities, we get

$$\frac{a^4V_{,\phi}^2}{4\mathcal{H}^2} \ll 2a^2V \Rightarrow a^2V_{,\phi}^2 \ll 8\mathcal{H}^2V. \tag{2.77}$$

From equation (2.73) we know that in this scenario the potential is dominating, which from the first Friedmann equation (2.38) tell us that

$$\mathcal{H}^2 = \frac{\kappa^2}{3}a^2V.$$

We insert this into our condition so that

$$V_{,\phi}^2 \ll \frac{8\kappa^2}{3}V^2, \tag{2.78}$$

or

$$\frac{3}{8\kappa^2}\left(\frac{V_{,\phi}}{V}\right)^2 \ll 1. \tag{2.79}$$

This prompts us to define a slow-roll parameter so that

$$\epsilon \equiv \frac{3}{8\kappa^2}\left(\frac{V_{,\phi}}{V}\right)^2, \tag{2.80}$$

making the above condition $\epsilon \ll 1$ if we want inflation to act as a cosmological constant.

However we also want inflation to end at some point. The condition for this leads to another slow-roll parameter. We find this slow-roll parameter using the constraint on $\ddot{\phi}$,

$$\ddot{\phi} \ll a^2 V_{,\phi}, \tag{2.81}$$

which is imposed on us by equation (2.73) and equation (2.75). Varying equation (2.76) with respect to time, we then find an expression for $\ddot{\phi}$,

$$\ddot{\phi} = -\left(a^2 V_{,\phi} + \frac{a^2}{2\mathcal{H}} V_{,\phi\phi}\dot{\phi}\right) = \frac{a^4}{4\mathcal{H}^2} V_{,\phi\phi} V_{,\phi} - a^2 V_{,\phi},$$

which inserted into equation (2.81) gives

$$\frac{a^2}{4\mathcal{H}^2} V_{,\phi\phi} V_{,\phi} \ll 2V_{,\phi}. \tag{2.82}$$

We now insert our expression for the Hubble parameter and we find our new slow-roll parameter,

$$\frac{3}{4\kappa^2}\frac{V_{,\phi\phi}}{V} \ll 1 \Rightarrow \eta = \frac{3}{4\kappa^2}\frac{V_{,\phi\phi}}{V}. \tag{2.83}$$

This second condition becomes $|\eta| \ll 1$. We also note that using the Friedmann equations together with these slow-roll approximations, we find that the first slow-roll parameter can also be written

$$\epsilon = -\frac{\dot{\mathcal{H}}}{\mathcal{H}^2}.$$

To recapitulate; in order to have an accelerating universe we need $\epsilon < 1$, and we consider the end of inflation to be the moment $\epsilon = 1$.

At the end of inflation, the scalar field will start oscillating about the minimum of the potential, and due to the friction term in equation (2.75) the scalar field will lose energy to the environment, damping the oscillations. This energy stored in the scalar field will therefore go into creating the particles of the Universe we recognize today. We call this process reheating. After reheating, the Universe evolves as a radiation dominated universe just as the Big Bang model says. One final, major point of inflation is that it sets up the initial perturbations, which will evolve into the first structures in the Universe, but in order to look at this, we need to know some perturbation theory.

2.7.4 Perturbation Theory

As mentioned, the standard Big Bang model utilizes the homogeneous and isotropic FLRW metric, and explains the evolution of matter using standard general relativity. But, as we know, an homogeneous model is not sufficient enough to explain the complex distribution of matter and energy we observe, everything from stars to galaxies to clusters to superclusters of galaxies, over a huge variation of scales. We need a model to describe an inhomogeneous and anisotropic universe, therefore we will use a perturbative approach starting with the FLRW model that works as a background solution, as demonstrated in Figure 2.2.

Choosing a set of coordinates in the inhomogeneous and anisotropic universe, which we as just mentioned will model with a FLRW background plus perturbations, require us to map spacetime points between the homogeneous background model and the inhomogeneous and anisotropic universe [18]. The freedom we get from doing this mapping is called the gauge freedom, or gauge issue, leading to apparently different descriptions of the same physical solution simply due to the choice of coordinates. This can be a powerful tool for us, as it allows us to work with variables best suited to our problem, but at the same time it leads to ambiguities in our choice of coordinates. This issue is expanded upon in Chapter 5.

In general we'll keep all perturbations to linear order, as progress gets much more difficult due to the non-linearity of the Einstein equations. Any tensor quantity with both spatial and time dependencies $A(\eta, x^i)$ can be split into a time-only dependent homogeneous background term and a time- and spatial dependent inhomogeneous perturbations as

$$A(\eta, x^i) = A(\eta) + \delta A(\eta, x^i). \tag{2.84}$$

We immediately employ this on the metric tensor,

$$g_{\mu\nu} = g^{(0)}_{\mu\nu} + h_{\mu\nu}, \tag{2.85}$$

where we use (0) to denote background quantity, and let $h_{\mu\nu} = \delta g_{\mu\nu}$ be the perturbation of the metric. It can then be split up into scalar, vector and tensor modes as,

$$h_{\mu\nu} dx^\mu dx^\nu = a(\eta)^2 \left(-2\Phi d\eta^2 + 2B_i d\eta dx^i + 2C_{ij} dx^i dx^j\right), \tag{2.86}$$

where $\delta g_{00} = -2a^2\Phi$ is a scalar quantity and Φ is known as the lapse, $\delta g_{0i} = a^2 B_i$ is a vector quantity and B_i is known as the shift, and for a scalar is interpreted as a partial derivative, and $\delta g_{ij} = 2a^2 C_{ij}$ is a tensor of rank 2; more on this in Appendix A. The nature of these components is technically what we mean when we choose between gauges - some of these components disappear for certain gauges, and some not. But before we take a look at gauges, let's see why we need perturbation theory.

Initial perturbations

One of the other problems with the traditional Big Bang model was that it called for a homogeneous universe, and if the Universe was completely homogeneous to begin with it would stay so forever. It turns out that from Heisenberg's uncertainty principle that inflation will start and end at different times for different regions of space, which will ultimately lead to primordial fluctuations during inflation.

We look at perturbations of the density as $\rho = \rho + \delta\rho$. Let us see how we can relate these to the scalar field of inflation. Consider a volume containing two elements with a total energy E. During inflation one of these elements is stretched by a factor a, while the other is stretched by $a + \delta a$. Finally, let $\delta a = \dot{a}\delta\eta$. This leads to a difference in the energy density after inflation of

$$\delta\rho = \frac{E}{a^3} - \frac{E}{(a+\delta a)^3} = \frac{E}{a^3}\left(1 - (1 + \mathcal{H}\delta\eta)^{-3}\right) \approx \rho\,(1 - (1 - 3\mathcal{H}\delta\eta)) = 3\mathcal{H}\rho\delta\eta, \quad (2.87)$$

where we used a Taylor approximation, so that

$$\frac{\delta\rho}{\rho} = 3\mathcal{H}\delta\eta. \quad (2.88)$$

If we now perturb the scalar field so that $\phi = \phi + \delta\phi$ we see that we can tweak this by using $\delta\phi = \dot{\phi}\delta\eta$ showing us that

$$\frac{\delta\rho}{\rho} = 3\mathcal{H}\frac{\delta\phi}{\dot{\phi}}, \quad (2.89)$$

and we see that small fluctuations in the scalar field will lead directly to perturbations in the density! This tells us that the scalar field driving inflation, that contain small fluctuations, will lead to density perturbations, which again will lead to matte being unevenly distributed in the Universe. This will lead to matter clustering, and eventually forming the first structures of the Universe.

2.7.5 Gravitational Waves

In the same manner that we have waves in electromagnetic fields, so should it be for the gravitational field according to general relativity. This is a unique prediction of GR, and has as of yet not been directly observed. However we can still find constraints on them to help future observational astronomers in detecting them. It turns out that the scalar field and its fluctuations during inflation is one potential source for these gravitational waves, and inflation can give us the expected amplitude of these gravitational waves. Or rather, inflation give us the ratio between the tensor and scalar amplitudes r [7]. We will return to this briefly in Chapter 7.

2.7.6 Gauges

With those short detours out of the way, let us return to discussing what components of the perturbed metric we shall keep.

Synchronous gauge

For most of the remainder of the thesis we will frequently be working in the synchronous gauge. We choose to work in this gauge mostly as it provides an unambiguous time coordinate, the lapse and shift components are both zero, it resembles a normal Minkowski spacetime with spatial dependencies added on, and most importantly, it is numerically stable. This is why most of the existing Boltzmann codes are written in this gauge. I present more on this in Chapter 6. However, synchronous gauge is also riddled with potential problems, which we discuss in depth soon.

The synchronous gauge is defined as,

$$ds^2 = a^2(-d\eta^2 + (\delta_{ij} + h_{ij})dx^i dx^j), \tag{2.90}$$

where $h_{ij} = 2\partial_i\partial_j E - 2\Psi\delta_{ij}$, where Ψ is a curvature term. With this gauge we get the following Christoffel symbols,

$$\begin{aligned}
\Gamma^0_{00} &= \mathcal{H}, \\
\Gamma^0_{ij} &= \mathcal{H}(\delta_{ij} + h_{ij}) + \frac{1}{2}\dot{h}_{ij}, \\
\Gamma^i_{j0} &= \mathcal{H}\delta^i_j + \frac{1}{2}\dot{h}^i_j, \\
\Gamma^i_{jk} &= \frac{1}{2}(\partial_k h^i_j + \partial_j h^i_k - \partial^i h_{jk}),
\end{aligned} \tag{2.91}$$

giving us a Ricci scalar of the form

$$R = \frac{1}{a^2}\left(6\frac{\ddot{a}}{a} + \ddot{h} + 3\mathcal{H}\dot{h} - \nabla^2 h + \partial_i\partial^i h^i_j\right), \tag{2.92}$$

where $h = h^i_i = \delta^{ij}h_{ij}$.

We also have ways to transform from any other gauge into the synchronous gauge by performing transformations. These transformations are found in [18]; however they also contain an unfixed constant $\mathcal{C}(x^i)$, as well as a general integral. In order to remove this ambiguity [19, 18, 20] we fix the synchronous gauge to cold dark matter. Since matter continuity implies that $\partial(av_c)/\partial\eta = 0$, where v_c is the velocity of CDM, in synchronous gauge [21], fixing the gauge to CDM at an initial time will fix it for all times. I present the fixed transformations, where we label synchronous gauge variables with the subscript *syn*:

$$\delta_{syn} = \delta - 3\mathcal{H}(1+w)v_c, \tag{2.93}$$

$$\Psi_{syn} = \Psi - \mathcal{H}v_c, \tag{2.94}$$

$$v_{syn} = v - v_c, \tag{2.95}$$

$$\dot{E}_{syn} = v_c, \tag{2.96}$$

$$\delta\psi_{syn} = \delta\psi + \dot{\psi}v_c. \tag{2.97}$$

Conformal Newtonian Gauge

Conformal Newtonian gauge is a safer gauge than the synchronous gauge, as we will see later, and it keeps aspects such as the gravitational potential from Newtonian physics in the line-element to make it much more intuitive. It is defined as

$$ds^2 = a^2(-(1+2\Phi)d\eta^2 + (1-2\Psi)\delta_{ij}dx^i dx^j), \tag{2.98}$$

where Φ is related to the gravitational potential from Newtonian physics. With this gauge we get the Christoffel symbols to first order,

$$\begin{aligned}
\Gamma^0_{00} &= \dot{\Phi} + \mathcal{H}, \\
\Gamma^0_{0i} &= \partial_i \Phi, \\
\Gamma^0_{ij} &= -\dot{\Psi}\delta_{ij} + \mathcal{H}(1 - 2(\Psi + \Phi))\delta_{ij}, \\
\Gamma^i_{00} &= \partial^i \Phi, \\
\Gamma^i_{j0} &= (\mathcal{H} - \dot{\Psi})\delta^i_j, \\
\Gamma^i_{jk} &= \partial^i \Psi \delta_{jk} - \partial_k \Psi \delta^i_j - \partial_k \Psi \delta^i_j,
\end{aligned} \tag{2.99}$$

giving us a Ricci scalar of the form

$$R = \frac{6}{a^2}\left((1-2\Phi)\frac{\ddot{a}}{a} - \mathcal{H}\dot{\Phi} - 3\mathcal{H}\dot{\Psi} - \ddot{\Psi}\right). \tag{2.100}$$

Similarly to how we can transform any gauge into the synchronous gauge, we can transform any gauge to conformal Newtonian gauge. We label conformal Newtonian gauge variables with the subscript N:

$$\Phi_N = \Phi + \mathcal{H}(B - \dot{E}) + \frac{\partial}{\partial \eta}(B - \dot{E}), \tag{2.101}$$

$$\Psi_N = \Psi - \mathcal{H}(B - \dot{E}), \tag{2.102}$$

$$\delta_N = \delta - 3\mathcal{H}(1+w)(B - \dot{E}), \tag{2.103}$$

$$v_N = v + \dot{E}, \tag{2.104}$$

$$\delta\psi_N = \delta\psi + \delta\dot{\psi}(B - \dot{E}). \tag{2.105}$$

Other Gauges

The above gauges are as already stated the most important ones for our purposes; however we still need to introduce at least two more. We will use these gauges in Chapter 5 and 6.

Spatially flat gauge: The spatially flat gauge is also called the uniform curvature gauge, and is a gauge where we have no scalar curvature perturbations at all, $\Psi = E = 0$. For more on the spatially flat gauge, I refer the reader once again to [18].

Uniform field gauge: The uniform field gauge is a gauge where the scalar field is homogeneous, meaning no scalar field perturbations, $\delta\psi = E = 0$. For more on the uniform field gauge, I refer the reader to [22].

Uniform density gauge: The density curvature gauge is a gauge that is completely homogeneous, with $\delta\rho = 0$ and either $E = 0$ or $B = 0$ as one are free to choose whichever is best suited for the situation at hand. For more on the uniform density gauge, I refer the reader to [18].

2.7.7 The Stress-Energy Tensor Revisited

Now that we have gauges defined, we can continue studying the stress energy tensor (2.14). By assuming the fluid we look at to be isotropic and barotropic so that $q = \pi_{\mu\nu} = 0$, we find the components of the stress-energy tensor in the synchronous gauge,

$$T^0_0 = -\rho, \quad T^i_0 = -(\rho + p)v^i, \quad T^i_j = p\delta^i_j, \tag{2.106}$$

where we chose to work in mixed form because this removes the h_{ij} terms. The stress-energy tensor obeys the conservation law,

$$\nabla_\mu T^\mu_\nu = \mathcal{C}_\nu, \tag{2.107}$$

where $\mathcal{C}_\nu$ is the collision term, representing occurrences such as momentum transfer between baryons and photons through Thomson scattering. Let us work out the conservation law to first order, remembering the conventions displayed in §1.1.3:

$$\begin{aligned}\nabla_\mu T^\mu_\nu = {} & \partial_0 T^0_\nu + \Gamma^0_{00} T^0_\nu + \Gamma^i_{0i} T^0_\nu + \Gamma^0_{s0} T^s_\nu + \Gamma^i_{si} T^s_\nu \\ & + \partial_i T^i_\nu - \Gamma^0_{0\nu} T^0_0 - \Gamma^0_{i\nu} T^i_0 - \Gamma^s_{0\nu} T^0_s - \Gamma^s_{i\nu} T^i_s.\end{aligned} \tag{2.108}$$

This gives us

$$\nabla_\mu T^\mu_0 = \partial_0 T^0_0 + \partial_i T^i_0 + \left(3\mathcal{H} + \frac{1}{2}\dot{h}\right) T^0_0 + \frac{1}{2}(\partial_i h^i_s + \partial_s h - \partial^i h_{is}) T^s_0 - \left(\mathcal{H}\delta^s_i + \frac{1}{2}\dot{h}^s_i\right) T^i_s \tag{2.109}$$

and

$$\nabla_\mu T^\mu_j = \partial_0 T^0_j + \partial_i T^i_j + \left(4\mathcal{H} + \frac{1}{2}\dot{h}\right) T^0_j - \left[(\delta_{ij} + h_{ij})\,\mathcal{H} + \frac{1}{2}\dot{h}_{ij}\right] T^i_0 - \left(\mathcal{H}\delta^s_j + \frac{1}{2}\dot{h}^s_j\right) T^0_s. \tag{2.110}$$

Remember that equation (2.106) is general for any perfect fluid that is isotropic and barotropic, and that most of the components in the Universe can be viewed as a fluid with a specific equation of state[17]. We can therefore find the equation of motion for any fluid by inserting equation (2.106) into equation (2.109) and equation (2.110),

$$\nabla_\mu T^\mu_0 = -\dot{\rho} - \partial_i((\rho+p)v^i) - (\rho+p)\left(3\mathcal{H} + \frac{1}{2}\dot{h}\right), \tag{2.111}$$

$$\nabla_\mu T^\mu_j = \frac{\partial}{\partial\eta}((\rho+p)v^i) - (\rho+p)\left(3\mathcal{H} + \frac{1}{2}\dot{h}\right). \tag{2.112}$$

Let us also perturb the system in the manner

$$\rho \to \rho + \rho\delta,\ p \to p + \delta p,\ \delta p = c_s^2\rho\delta, \tag{2.113}$$

where we introduced a new way of perturbing the density, by using the dimensionless perturbation $\delta = \frac{\delta\rho}{\rho}$. We'll also need to perturb the right hand side of the conservation law, so we set $\mathcal{C}_\nu \to \mathcal{C}_\mu + \delta\mathcal{C}_\mu$. Equation (2.111) then gives us

$$\dot{\rho} + 3\mathcal{H}\rho(1+w) = -\mathcal{C}_0 \tag{2.114}$$

for the background, and

$$\dot{\delta} + (1+w)\left[\partial_i v^i + \frac{1}{2}\dot{h}\right] + 3\mathcal{H}(c_s^2 - w)\delta = \delta\mathcal{C}_0 \tag{2.115}$$

for the perturbations. Likewise from equation (2.112) we get

$$\partial_j p = 0 \tag{2.116}$$

and

$$\dot{v}_j + \frac{c_s^2}{1+w}\partial_j\delta + \left[\frac{\dot{w}}{1+w} + \mathcal{H}(1-3w)\right]v_j = \delta\mathcal{C}_j. \tag{2.117}$$

2.8 Observations

As mentioned a couple of times throughout the thesis so far, it is possible to directly measure certain parameters, while others can be deduced from other observations. From the redshift of distant galaxies, we can estimate the present day value of the Hubble parameter, which today is thought to be $\mathcal{H}_0 = 100h$ km(sMpc)$^{-1}$ where $h = 0.7$. The density parameters of baryons, cold dark matter and dark energy are found from analyzing the WMAP 7-year data [24], estimated to be about $\Omega_{b0} = 0.04$, $\Omega_{m0} = 0.23$ and $\Omega_{\Lambda 0} = 0.73$.

[17]From the photon to the scalar field, everything can be viewed as a fluid [23]. However let us remark that photons can only be considered a fluid before "tight-coupling" breaks down, while neutrinos technically can never be considered a fluid, but the literature makes arguments that the error is negligible for neutrinos today.

2.8.1 The Power Spectrum

We've talked about the CMB being an observation of the photons released from decoupling, while in fact what we observe are temperature fluctuations. These temperature fluctuations are observed on a spherical surface, and can therefore be written as a sum of spherical harmonic functions,

$$\frac{\delta T}{T}(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm} Y_{lm}(\theta,\phi), \tag{2.118}$$

where Y_{lm} are the spherical harmonics, a_{lm} are the spherical harmonic coefficients, l is the angular scale tied with the wavenumber $k \sim l^{-1}$ so that a higher l represents a smaller scale, and θ and ϕ are of course the polar coordinates over which we measure the CMB. We now introduce the angular power spectrum C_l as the expectation value of the spherical harmonic coefficients,

$$C_l \equiv \langle |a_{lm}|^2 \rangle = \langle a_{lm} a_{lm}^* \rangle = \frac{1}{2l+1} \sum_{m=-1}^{l} |a_{lm}|^2. \tag{2.119}$$

From this it is obvious that we need an expression for a_{lm}, so we simply invert the above equation so that

$$a_{lm} = \int_{\Omega} \frac{\Delta T}{T}(\theta,\phi) Y_{lm}^*(\theta,\phi) d\Omega. \tag{2.120}$$

Fourier space

In order to simplify the equations, we choose to work in Fourier space, where the derivatives take on a much simpler form. For a quantity $A(\eta, \boldsymbol{x})$ the Fourier transform look like

$$A(\eta,\boldsymbol{x}) = \frac{1}{(2\pi)^3} \int d^3\boldsymbol{k} A(\eta,\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}, \tag{2.121}$$

$$A(\eta,\boldsymbol{k}) = \int d^3\boldsymbol{x} A(\eta,\boldsymbol{x}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{2.122}$$

This might look convoluted, but it boils down to letting $\frac{d}{dx} \rightarrow -i\boldsymbol{k}\cdot\mathbf{x}$, simplifying everything immensely. From now on all quantities are in Fourier space unless otherwise stated.

For a general quantity $\xi(\hat{\mathbf{k}})$ that quantify the statistics of a perturbation, be it temperature, density, curvature or whatever perturbations, the primordial power spectrum is defined through the two-point correlation function,

$$\langle \xi(\hat{\mathbf{k}}) \xi^*(\hat{\mathbf{k}}) \rangle = \frac{2\pi^2}{k^3} \mathcal{P}(k)\, \delta(\mathbf{k}-\mathbf{k}')(2\pi)^3. \tag{2.123}$$

From equation (2.120) the CMB angular power spectrum can also be defined, when for instance viewing a curvature perturbation $\xi(\boldsymbol{k}) = \mathcal{R}(\boldsymbol{k})$, as

$$C_l = \frac{1}{8\pi}\int_k \mathcal{P}_{\mathcal{R}}(k)\,|\Delta_{Tl}(k,\eta_0)|^2\,\frac{dk}{k}, \tag{2.124}$$

where the Δ_{Tl} is a so-called photon brightness function; similar forms hold for polarization.

2.8.2 Bispectrum

The bispectrum is conceptually the same as the power spectrum, in three-dimensions instead of one, and can also be found by using the spherical harmonic coefficients,

$$B_{l_1l_2l_3} \equiv \langle a_{l_1m}a_{l_2m}a_{l_2m}\rangle \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \tag{2.125}$$

where

$$\begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{2.126}$$

is the Wigner 3-J symbol. The primordial bispectrum[18] $\mathcal{B}$ is found by using the three-point correlation function given as,

$$\langle \mathcal{R}(\boldsymbol{k}_1)\mathcal{R}(\boldsymbol{k}_2)\mathcal{R}(\boldsymbol{k}_3)\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3)\mathcal{B}(k_1,k_2,k_3). \tag{2.127}$$

The CMB angular bispectrum is given [25, 26] by

$$\begin{aligned} B_{l_1l_2l_3} = {} & \left(\frac{2}{\pi}\right)^3 \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \\ & \times \int (k_1k_2k_3)^2 \mathcal{J}_{l_1l_2l_3}\mathcal{B}(k_1,k_2,k_3)\Delta_{l_1}(k_1)\Delta_{l_2}(k_2)\Delta_{l_3}(k_3)dk_1dk_2dk_3, \end{aligned} \tag{2.128}$$

where

$$\mathcal{J}_{l_1l_2l_3} = J_{l_1l_2l_3}(k_1,k_2,k_3) = \int j_{l_1}(k_1x)j_{l_2}(k_2x)j_{l_3}(k_3x)x^2dx. \tag{2.129}$$

It is common [26] to work instead with the reduced bispectrum,

$$\hat{B}_{l_1l_2l_3} = \left(\frac{2}{\pi}\right)^3 \int (k_1k_2k_3)^2 \mathcal{J}_{l_1l_2l_3}\mathcal{B}(k_1,k_2,k_3)\Delta_{l_1}(k_1)\Delta_{l_2}(k_2)\Delta_{l_3}(k_3)dk_1dk_2dk_3. \tag{2.130}$$

[18] Primordial is used to denote anything that was set up at the end of inflation. Primordial bispectrum is thus the bispectrum as it looked at the end of inflation.

The same forms hold for the temperature and polarization correlations. This leaves us with the problem of a triple-integral across a wildly-oscillating function, and the convoluted term $J_{l_1 l_2 l_3}$ which can be further studied at [27].

However luckily for us, an alternative approach to calculate the integral across Bessel functions is provided by Mehrem, Lindergant and Macfarlane in [28]. In this approach they find a way to evaluate integrals of the form

$$I(l_1 l_2 ... l_n; k_1 k_2 ... k_n) = \int_0^\infty x^2 dx \prod_{i=1}^{n} j_{l_i}(k_i x), \tag{2.131}$$

which we see is exactly the same as our definition of the Bessel function $\mathcal{J}_{l_1 l_2 l_3}$ in equation (2.129). By closely following their paper [28] we introduce a quantity

$$\Delta = \frac{k_1^2 + k_2^2 + k_3^2}{2k_1 k_2}, \tag{2.132}$$

that lies between ± 1, and can be interpreted as the cosine of the angle between $\hat{k_1}$ and $\hat{k_2}$ in the triangle formed by $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ and $\boldsymbol{k}_3$, see Figure 2.3 With

$$\Theta(\Delta) = \vartheta(1 - \Delta)\vartheta(1 + \Delta), \tag{2.133}$$

where

$$\begin{aligned} \vartheta(y) &= 0 \quad \text{for} \quad y < 0, \\ \vartheta(y) &= \frac{1}{2} \quad \text{for} \quad y = 0, \\ \vartheta(y) &= 1 \quad \text{for} \quad y > 0. \end{aligned}$$

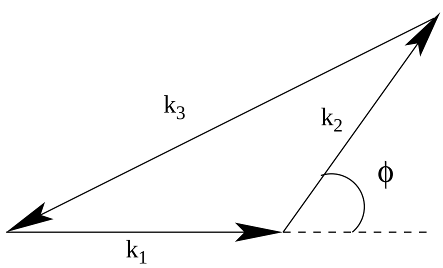

Figure 2.3: The triangle configuration formed by $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ and $\boldsymbol{k}_3$. This triangle formation ensures statistical isotropy.

With this and some relations to Legender polynomials P_l [28] they rewrite the integral (2.131) to obtain

$$
\begin{aligned}
J_{l_1 l_2 l_3}(k_1, k_2, k_3) = \frac{\pi \Theta(\Delta)}{4 k_1 k_2 k_3} & i^{l_1+l_2-l_3} \sqrt{2l_3+1} \left(\frac{k_1}{k_3}\right)^{l_3} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}^{-1} \\
& \cdot \sum_{\mathcal{L}=0}^{l_3} \binom{2l_3}{2\mathcal{L}}^{1/2} \left(\frac{k_2}{k_1}\right)^{\mathcal{L}} \sum_l (2l+1) \begin{pmatrix} l_1 & l_3-\mathcal{L} & l \\ 0 & 0 & 0 \end{pmatrix} \\
& \cdot \begin{pmatrix} l_2 & \mathcal{L} & l \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_1 & l_2 & l_3 \\ \mathcal{L} & l_3-\mathcal{L} & l \end{Bmatrix} P_l(\Delta),
\end{aligned}
\tag{2.134}
$$

where the new term is a Wigner 6-J symbol. It is worth noting that $l_1 + l_2 + l_3$ is always an even number, so that the integral will always stay real. With this approach we can evaluate our bispectrum without having to deal with the integrals themselves, and rather calculate the Wigner symbols using routines from the GNU Scientific Library [29]. Also note that we have a an infinite sum in equation (2.134), however we know that for the Wigner 3-J symbol of the form (2.126), with $m_1 = m_2 = m_3 = 0$, that $|l_1 - l_2| \leq l_3 \leq |l_1 + l_2|$, and is otherwise zero. From this we can find an upper limit to our sum as either $l_{\max} = |l_1 + l_3 - \mathcal{L}|$ or $l_{\max} = |l_2 + \mathcal{L}|$, whichever is smallest.

Chapter 3

Introduction to $f(R)$ Gravity

$f(R)$ gravity is one of many variations of Einstein's gravity model, which we focus on since some $f(R)$ models can explain the accelerated expansion of the Universe without introducing new exotic particles as the source of dark matter and dark energy, as well as providing a robust toy model for pushing the limit of our existing theories. For even more details on $f(R)$ theory than what we provide here, see [10, 30, 31] and their references. Aspects of this chapter are found in our paper [1].

3.1 Jordan Frame

As mentioned, in $f(R)$ theory the Einstein-Hilbert Lagrangian density is replaced with a general function of the Ricci scalar, so the action takes the form,

$$S = \frac{1}{2\kappa^2} \int d^4x \sqrt{-g} f(R) + \int d^4x \mathcal{L}_M \left(g_{\mu\nu}, \Psi_M \right) \tag{3.1}$$

where Ψ_M denotes the matter fields. The field equations follow by varying this action with respect to the metric as we did in §2.4.5,

$$FR_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} - \nabla_\mu \nabla_\nu F + g_{\mu\nu} \nabla^\alpha \nabla_\alpha F = \kappa^2 T^{(M)}_{\mu\nu}, \quad T^{(M)}_{\mu\nu} = -\frac{2}{\sqrt{-g}} \frac{\delta \mathcal{L}_M}{\delta g^{\mu\nu}}. \tag{3.2}$$

Here $F = \partial f / \partial R$. If we assume that there are no particles/fields interacting, the collision term $\mathcal{C}_\mu = 0$, and the conservation law equation (2.107) for the matter stress-energy tensor is

$$\nabla^\mu T^{(M)}_{\mu\nu} = 0. \tag{3.3}$$

This form of the theory is known as the "Jordan Frame", and in this frame the flat FLRW metric is exactly as provided earlier

$$ds^2 = a^2(\eta) \left(-d\eta^2 + \delta_{ij} dx^i dx^j \right). \tag{3.4}$$

3.1.1 Equivalence with Brans-Dicke Theory

By introducing a new auxiliary field ξ it can be shown [10, 32] that $f(R)$ theory can be cast as Brans-Dicke theory with $\omega_{\text{BD}} = 0$ so long as $\partial^2 f/\partial R^2 \neq 0$. We see this by adding the new field ξ to the action (3.1),

$$S = \frac{1}{2\kappa^2}\int d^4x\sqrt{-g}\left[f(\xi) + f_{,\xi}(\xi)(R-\xi)\right] + \int d^4x\mathcal{L}_M\left(g_{\mu\nu}, \Psi_M\right), \tag{3.5}$$

and then varying this with respect to the new field ξ to get

$$f_{,\xi\xi}(R-\xi) = 0.$$

If we impose that $f_{,\xi\xi} \neq 0$, we see that we must have $R = \xi$, so that the action returns to the form of equation (3.1). If we now introduce yet another field,

$$\phi \equiv f_{,\xi}, \tag{3.6}$$

then we can rewrite equation (3.5) to the form

$$S = \int d^4x\sqrt{-g}\left[\frac{1}{2\kappa^2}\phi R - U(\phi)\right] + \int d^4x\mathcal{L}_M\left(g_{\mu\nu}, \Psi_M\right), \tag{3.7}$$

where we have set

$$U(\phi) = \frac{\xi\phi - f(\xi)}{2\kappa^2}. \tag{3.8}$$

Why we rewrote the action like this is immediately clear when we compare it to the action in Brans-Dicke theory with a potential $U(\phi)$ [10, 33],

$$S = \int d^4x\sqrt{-g}\left[\frac{1}{2\kappa^2}\phi R - \frac{\omega_{BD}}{2\phi}(\nabla\phi)^2 - U(\phi)\right] + \int d^4x\mathcal{L}_M\left(g_{\mu\nu}, \Psi_M\right), \tag{3.9}$$

which we see is equal to equation (3.7) if we set $\omega_{BD} = 0$. With the Brans-Dicke representation $f(R)$ theory has also been described and studied as an example of "extended quintessence" (e.g. [34] and its references).

3.1.2 Jordan Frame in Synchronous Gauge

With the Einstein field equations (3.2) for $f(R)$ gravity in the Jordan Frame safe in hand, let us see what they look like in the synchronous gauge. Remembering synchronous gauge,

$$ds^2 = a^2(\eta)\left(-d\eta^2 + \left(\delta_{ij} + h_{ij}\right)dx^i dx^j\right), \tag{3.10}$$

where it is worth noting that the inverse of g_{ij} is $a^2 g^{ij} = \delta^{ij} - h^{ij}$, we get,

$$3\mathcal{H}^2 - 3\frac{\ddot{a}}{a} + \frac{a^2}{2}\frac{f}{F} + 3\mathcal{H}\frac{\dot{F}}{F} = \frac{\kappa^2 a^2\rho}{F}, \tag{3.11}$$

$$\frac{\ddot{a}}{a} + \mathcal{H}^2 - \frac{a^2}{2}\frac{f}{F} - \frac{\ddot{F}}{F} - \mathcal{H}\frac{\dot{F}}{F} = \frac{\kappa^2 a^2 p}{F}, \tag{3.12}$$

for the background and

$$\frac{1}{2}\dot{h}\dot{F} - \frac{F}{2}\left(\ddot{h} + \mathcal{H}\dot{h}\right) - \nabla^2 F + h^{ij}\partial_i\partial_j F + \frac{1}{2}\left(2\partial^i h_i^s - \partial^s h\right)\partial_s F = a^2\kappa^2\delta\rho, \tag{3.13}$$

$$\left[F\left(\frac{\ddot{a}}{a} + \mathcal{H}^2\right) - \frac{1}{2}a^2 f - \ddot{F} + \nabla^2 F - \mathcal{H}\dot{F}\right] h_{ij} + \frac{1}{2}F\ddot{h}_{ij} + \dot{h}_{ij}\left(\mathcal{H}F + \frac{1}{2}\dot{F}\right)$$
$$+ \dot{h}\left(\frac{1}{2}\mathcal{H}F\delta_{ij} - \frac{1}{2}\dot{F}\delta_{ij}\right) - \frac{1}{2}\left(\nabla^2 h_{ij} + \partial_i\partial_j h - \partial_a\partial_i h_j^a - \partial_j\partial^a h_{ia}\right)F - \delta_{ij}h^{kl}\partial_l\partial_k F$$
$$+ \frac{1}{2}\left(\partial_j h_i^s + \partial_i h_j^s - \partial^s h_{ij} + \delta_{ij}\left(\partial^s h - 2\partial^l h_l^s\right)\right)\partial_s F = \kappa^2 a^2 h_{ij} p, \tag{3.14}$$

for the perturbations.

3.2 Einstein Frame

We utilize the transformation rules set down in §2.5.2, and by writing $f = RF + (f - RF) = RF - U$, the action (3.1) can then be rewritten as

$$S = \int \sqrt{-\tilde{g}}\left[\frac{F}{2\kappa^2\Omega^2}\left(\tilde{\rho} + 6\tilde{\nabla}^\mu\tilde{\nabla}_\mu\omega - 6\tilde{\nabla}^\mu\omega\tilde{\nabla}_\mu\omega\right) - \frac{U}{\Omega^4}\right]d^4x \tag{3.15}$$
$$+ \int \mathcal{L}_M\left(\Omega^{-2}\tilde{g}_{\mu\nu}, \Psi_M\right)d^4x.$$

The Einstein frame is then defined by isolating a Ricci scalar in the action to serve as the Einstein-Hilbert Lagrangian density; this can be found by choosing

$$\Omega^2 = F \tag{3.16}$$

which requires the condition $F > 0$ to be always satisfied. Casting the rest of the action into the form of a scalar field minimally-coupled to gravity,

$$\kappa^2\tilde{\phi} = -\frac{1}{2Q}\ln F, \qquad Q = -\frac{1}{\sqrt{6}}, \tag{3.17}$$

produces[1]

$$S = \int \sqrt{-\tilde{g}}\left(\frac{1}{2\kappa^2}\tilde{R} - \frac{1}{2}\tilde{\nabla}^\mu\tilde{\phi}\tilde{\nabla}_\mu\tilde{\phi} - \tilde{V}(\tilde{\phi})\right)d^4x + S_M\left(e^{2Q\kappa\tilde{\phi}}\tilde{g}_{\mu\nu}, \Psi_M\right), \tag{3.18}$$

where $\tilde{V}(\tilde{\phi}) = \dfrac{U}{2\kappa^2 F}$.

This action describes general relativity in the presence of a scalar field minimally-coupled to gravity but non-minimally coupled to matter – an example of a "coupled

[1] The term $\nabla^\mu\nabla_\mu\omega$ disappears due to Gauss' theorem.

quintessence" (e.g. [34, 35, 36, 37, 38, 39]) model[2]. The stress-energy tensor and potential of the scalar field are

$$\tilde{T}^{(\phi)}_{\mu\nu} = \tilde{\nabla}_\mu\tilde{\phi}\tilde{\nabla}_\nu\tilde{\phi} - \frac{1}{2}\tilde{g}_{\mu\nu}\tilde{\nabla}^\sigma\tilde{\phi}\tilde{\nabla}_\sigma\tilde{\phi} - \tilde{V}(\tilde{\phi})\tilde{g}_{\mu\nu}, \tag{3.19}$$

$$\tilde{V}(\tilde{\phi}) = \frac{RF - f}{2\kappa^2 F^2}. \tag{3.20}$$

By varying the action (3.18) with respect to the field ϕ we find a new version of the Klein Gordon equation, giving us a new equation of motion for the field, as

$$\tilde{\Box}\tilde{\phi} - \frac{\partial\tilde{V}}{\partial\tilde{\phi}} = -\frac{1}{\sqrt{-\tilde{g}}}\frac{\partial\mathcal{L}_M}{\partial\tilde{\phi}} = -\kappa Q\tilde{T}^{(M)}. \tag{3.21}$$

For further details see for example [10]. The flat FLRW metric in the Einstein frame is

$$d\tilde{s}^2 = \tilde{a}^2(\eta)\left(-d\eta^2 + \delta_{ij}dx^i dx^j\right) \tag{3.22}$$

where the coordinates are the same in the Einstein frame as in the Jordan frame – this is only possible because we are employing conformal instead of coordinate time!

3.2.1 Einstein Frame in Synchronous Gauge

In order to find the Einstein field equations in the Einstein frame, we can utilize all the transformations listed above in §2.5.2 on equations (3.13) - (3.14). However as the Einstein frame is a representation of standard general relativity, all we need to do is choose f and F to represent GR, which is; $f = \tilde{R}$, $F = 1$, $\dot{F} = \ddot{F} = 0$ so that we get

$$\begin{aligned} 3\tilde{\mathcal{H}}^2 - 3\frac{\ddot{\tilde{a}}}{\tilde{a}} + \frac{1}{2}\tilde{a}^2\tilde{R} &= \kappa^2\tilde{a}^2\tilde{\rho}, \\ \frac{\ddot{\tilde{a}}}{\tilde{a}} + \tilde{\mathcal{H}}^2 - \frac{1}{2}\tilde{a}^2\tilde{R} &= \kappa^2\tilde{a}^2\tilde{p}, \end{aligned} \tag{3.23}$$

for the background, where if we insert the Ricci scalar we found earlier $\tilde{R} = \frac{6}{\tilde{a}^2}\frac{\ddot{\tilde{a}}}{\tilde{a}}$, we would recover the Friedmann equations from standard GR, and

$$\ddot{h} + \mathcal{H}\dot{h} = -2\kappa^2 a^2\delta\rho, \tag{3.24}$$

$$\begin{aligned} \left[\left(\frac{\ddot{a}}{a} + \mathcal{H}^2\right) - \frac{1}{2}a^2\tilde{R}\right]h_{ij} + \frac{1}{2}\ddot{h}_{ij} + \mathcal{H}\dot{h}_{ij} - \frac{1}{2}\left(\nabla^2 h_{ij} + \partial_i\partial_j h - \partial_a\partial_i h^a_j - \partial_j\partial^a h_{ia}\right) \\ + \frac{1}{2}\mathcal{H}\dot{h}\delta_{ij} - \delta_{ij}h^{kl}\partial_l\partial_k = \kappa^2 a^2 h_{ij} p, \end{aligned} \tag{3.25}$$

for the perturbations.

[2] However, it should be noted that more recent coupled quintessence models such as that in [38] tend to couple the scalar field only to one species of matter, and do not easily, if at all, admit a Jordan frame representation.

3.3 The Equivalence Between the Frames

The meaning of this "equivalence" has a tangled history in the literature, the usage of which can be generally separated into two camps (see for example [13], who identify a number of works to that date with one camp or the other, and [15] which sets out clear definitions of "equivalence"): it can be taken to imply that the physics in both frames is identical, or it can be taken to imply that a system set up in the Jordan frame can be solved in the Einstein frame as long as it is transformed back to the Jordan frame for interpretation. The former case relies on us clearly stating what "physical equivalence" means; in [14] (and, similarly [40]) the authors take the reasonable definition that the observables should remain the same. The latter case requires us to define the concept of the "physical frame", the one in which observations should be taken. This would be the frame in which it is natural to define our theory; if we are motivated, as in $f(R)$ gravity, by a modification of the Einstein-Hilbert action then the Jordan frame would be the physical frame. If instead we were motivated, as in coupled quintessence, by exotic couplings between a scalar field and matter, then the Einstein frame would be the physical frame.

Particularly clear discussions of this issue is found in [13, 9] and for some time it seems generally agreed that the "equivalence" is at least mathematical in nature, but since it occasionally reappears in the literature (see for instance [40, 41, 42, 43, 44, 45, 46, 14, 15] for some examples since 2004) we briefly re-address the question here.

"Physical equivalence" between the frames implies that the general behaviour of solutions in the two frames would coincide. While the causal structure is naturally preserved by the conformal transformation, it is straightforward to find models with very different behaviours. For example, in polynomial gravity with $f(R) = \alpha R^n$ one can find [47] a dust-dominated cosmology with

$$a \propto \eta^{-2n/(2n-3)}, \quad \tilde{a} \propto \eta^{(n-3)/(2n-3)} \tag{3.26}$$

in the Jordan and Einstein frames respectively. The deceleration parameter (2.67), is then

$$q = \frac{1}{2}\left(\frac{3-2n}{n}\right), \quad \tilde{q} = \frac{2n-3}{n-3}. \tag{3.27}$$

The Universe in the Jordan frame is then accelerating if $n > 3/2$, but is accelerating in the Einstein frame if $n \in (3/2, 3)$. Choosing $n = 4$ gives $q = -5/8$ and $\tilde{q} = 5$. In the first case the Universe is accelerating, while in the second it is decelerating. In this strict respect, the frames are clearly not physically equivalent. This example is similar to that in [46]; extreme forms are presented in [42, 43] where the authors find a phantom behaviour[3] in one frame but a non-phantom frame in the other, and in [45] where a model based on a non-minimally coupled scalar field exhibits a bouncing behaviour in the Jordan frame but not in the Einstein frame.

[3] A phantom behaviour is simply a universe model with $w < -1$, violating all the established rules of GR.

In the previous section the two frames are shown to be mathematically equivalent at the level of the action. It is quick to confirm that the field equations in the two frames are also equivalent to one another, in that a solution in the Jordan frame maps directly onto a solution in the Einstein frame and vice-versa. Let's look at the Einstein equations in the Einstein frame,

$$\tilde{R}_{\mu\nu} - \frac{1}{2}\tilde{g}_{\mu\nu}\tilde{R} = \kappa^2\left(\tilde{T}^{(M)}_{\mu\nu} + \tilde{T}^{(\phi)}_{\mu\nu}\right), \tag{3.28}$$

and apply the transformations (2.28) and the form of the scalar field stress-energy tensor (3.20) to this:

$$\begin{aligned} R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R - 2\nabla_\alpha\nabla_\beta\omega + 2g_{\alpha\beta}\nabla^\mu\nabla_\mu\omega - 4\nabla_\alpha\omega\nabla_\beta\omega + 4g_{\alpha\beta}\nabla^\mu\omega\nabla_\mu\omega \\ = \kappa^2\Omega^{-2}T_{\alpha\beta} + \kappa^2\tilde{V}(\tilde{\phi})\Omega^2 g_{\alpha\beta}. \end{aligned} \tag{3.29}$$

Using now that $F = \Omega^2 > 0$ and $2\Omega^4\kappa^2\tilde{V} = \Omega^2 R - f(R)$ produces the field equations in the Jordan frame (3.2). Since the transformation is invertible, the reverse naturally follows. It is then trivial to show that any solution of the field equations in the Jordan frame induces a solution in the Einstein frame, and vice-versa: the two frames are equivalent, even if only one frame is "physical" in the sense defined above. See for example [11, 12, 13, 14] for other discussions and interpretations. For our purposes it suffices to take that the equivalence is mathematical and that observations should be made in the Jordan frame. This satisfies the interpretations of both camps.

While it is common to employ a general parametrization [48, 49, 50, 51] in the Jordan frame, working in the Einstein frame (e.g. [52, 53]) provides a flexible alternative. Exploiting the Einstein frame allows us to consider any modified gravity model which possesses an Einstein frame and for which background solutions in the Jordan frame might be extremely difficult to find, either analytically or numerically. It allows us to import our intuition and understanding from standard gravity – at least while we remain in the Einstein frame – and, perhaps more importantly, it allows us to directly leverage well-tested codes developed for general relativity and which contain a wealth of physics and arbitrary collections of fluids that would be extremely lengthy to implement in the Jordan frame, and it provides the added guarantee that we need evolve only second order rather than fourth order differential equations – a significant calculational simplification.

3.4 Various f(R) Models

In this section, we'll take a look at some selected $f(R)$ models, and shortly discuss how viable they are. By viable, we will here mean that they allow for a radiation dominated universe in the past and a matter domination at later time. Tight constraints on $f(R)$ models that give a viable matter-dominated phase are presented in [54] by Amendola and Tsujikawa, though these constraints only apply around the matter domination era. However at a classical level we are always free, for instance, to add a term αR^2 or $-\mu^4/R$ so long as α and μ are chosen such that the corrections do not break the conditions. To our knowledge, a comparable study constraining the transition from radiation domination to matter domination has not been performed in general.

3.4.1 $f(R) = R + \alpha R^2$

This theory of $f(R)$, $f(R) = R + \alpha R^2$, was the first model of inflation introduced by Starobinsky in 1979 [55], and is still the most realistic $f(R)$ theory. It is generally introduced as any power of R as $f(R) = R + \alpha R^n$; however as shown by Hwang and Noh in [56], $n \approx 2$ is the only viable option after they introduced the model $f(R) = R + \alpha R^{2+\epsilon}$ and found $\epsilon \ll 1$ when employing results from COBE. The αR^2 term leads to an accelerated expansion of the Universe, while the presence of the linear term R ensures that inflation will end gracefully [10]. It has been shown that this model is consistent with the temperature anisotropies observed by the CMB, and is actually a viable $f(R)$ theory and an alternative to scalar field inflation. For realistic values it is worth noting that this theory is equivalent to the concordance model with a $m_{Pl}^2\phi$ potential [56].

3.4.2 $f(R) = R - \frac{\mu^4}{R}$

This model, $f(R) = R - \mu^4/R$, was introduced by Carroll et. al. [57] and is an unstable solution [58]. It is plagued by matter instabilities, and fails to satisfy local gravity constraints, see [10] and references. Also, due to a strong coupling between dark energy and dark matter in this model it does not have a standard matter-dominated epoch. However, if μ is tuned to be small enough, it can be employed phenomenologically to model dark energy.

3.4.3 Other Models

If we combine the two above models, and add in a cosmological constant, we get $f(R) = -\mu^4/R - 2\Lambda + R + \alpha R^2$. This combination will drive an initial inflationary period, and then a late-time accelerating expansion, just as we would want. It however does not satisfy the Amendola and Tsujikawa bounds [54], so it is not a viable model for modified gravity. It can also be viewed as the leading order terms in the Laurent series [59] of a more general model. This model was proposed by Nojiri and Odintsov [60].

Alternatively we can do a leap and define, as presented by Appleby and Battye [61],

$$f(R) = \frac{1}{2}R + \frac{1}{2b}\log[\cosh(bR) - \tanh(c)\sinh(bR)], \tag{3.30}$$

where b and c are free parameters. This model satisfies the tight constraints on $f(R)$ models, and represents perhaps our most interesting model. However little work has been done on this model so far, so we don't have much more to say at this point and leave its study to future work. Appleby and Battye together with Starobinsky further expanded upon this model in [62].

Of all the models we've looked at, only the last is genuinely a "viable" modification to gravity in that it possesses a satisfactory matter-dominated era that transitions to an accelerating epoch. However, all of these models can be tweaked to be useful for our later purpose in Chapter 6.

3.5 The Palatini Approach

The Palatini approach is an alternative way of studying $f(R)$ gravity and is popular in cosmology (e.g. [63, 9, 64] and their references) and often employed in studies of cosmological perturbations (e.g. [65, 66, 31]). The approach differs from the metric approach we employ above, in that the Christoffel symbols are considered independent of the metric when we vary the action. This difference give rise to a different set of field equations. It is of note that the Palatini approach is equivalent with the Brans-Dicke theory with $\omega_{BD} = -3/2$. For more on the Palatini approach, see [10] and its references.

3.6 Honorable Mentions: Alternative Theories

3.6.1 The Chameleon Model

The Chameleon model was first introduced by Khoury and Weltman [67], and is a modified gravity theory where the scalar field has a mass that depends on the local matter density. This allows the Chameleon field to have a large mass in regions of high density, such as the solar system, while at the same time being very small at interstaller regions. These characteristics allow the chameleon model to affect regions at larger scales, while also leaving the local regions invariant to GR. I refer the reader to the master thesis of Hans Winther [68] for a great review. Also note that some $f(R)$ models can act as a Chameleon model.

3.6.2 Coupled Quintessence

Coupled quintessence has been mentioned several times in this thesis so far, and it is simply the way to describe a scalar field that is coupled to matter, unlike normal quintessence which is just a scalar field minimally coupled to matter, as we have used it above in our discussion of inflation. It however has the advantage that the field equations are only second order. For more on coupled quintessence, I refer the reader to [35].

3.6.3 Galileon

The Galileon model is in short a generalization of the DGP model. The DGP model [69] assumes that Minkowski space doesn't consist of 3+1 dimensions, but rather 4+1 dimensions. It uses an action consisting of the standard Einstein-Hilbert action in 4 dimensions, as it was portrayed in §2.16, and another action that is equivalent to the Einstein-Hilbert action in five dimensions. It assumes that the 4 dimensional part dominates on local scales, while the five dimensional part is dominates at large scales. As mentioned, the Galileon model is a generalization of this, for more on the Galileon model itself I refer the reader to [70].

3.6.4 Symmetron

The symmetron model hinges on a symmetry mechanism that is dependent on the local density. In regions with high matter density, the field in the symmetron model tends towards zero and its coupling to matter vanishes. In regions with low density, the symmetry is broken and the symmetron field couple to matter with gravitational strength. For mere on the symmetron model, I refer the reader to [71].

Chapter 4

The Statistics of an $f(R)$ Model

This chapter will for the most follow the paper by Tsujikawa and De Felice [2]; however it has been reformulated to fit our needs.

4.1 The Action and Background Equations

Any $f(R)$ model can be cast as an action on the form

$$S = \int d^4x\sqrt{-g}\left[\frac{m_{Pl}^2}{2}\phi R - U\right], \tag{4.1}$$

as showed in §3.1.1. By varying equation (4.1) with respect to the metric $g^{\mu\nu}$ and the scalar field ϕ, as described in §2.4.5, we find the field equation and continuity equation respectively,

$$\phi R_{\mu\nu} - \frac{\phi}{2}Rg_{\mu\nu} - \nabla_\mu\nabla_\mu\phi + g_{\mu\nu}\Box\phi + \frac{U}{m_{Pl}^2}g_{\mu\nu} = 0, \tag{4.2}$$

$$3m_{Pl}^2\Box\phi + 2U - U_{,\phi} = 0. \tag{4.3}$$

Note that we are in this section working in a vacuum filled, pressureless universe so that $T_{\mu\nu} = 0$.

Taking the 00 term and ij term of equation (4.2) we find the first two background equations,

$$E_1 = 3m_{Pl}^2\left(\mathcal{H}\dot{\phi} + \mathcal{H}^2\phi\right) - a^2U = 0, \tag{4.4}$$

$$E_2 = m_{Pl}^2\left(\mathcal{H}^2\phi + 2\frac{\ddot{a}}{a}\phi + 2\mathcal{H}\dot{\phi} + \ddot{\phi}\right) - a^2U = 0. \tag{4.5}$$

By then either expanding out equation (4.3) using relations described in §2.4.5, or simply by combining equation (4.4) and equation (4.5) with the Bianchi identity,

$$\dot{\phi}E_3 = -3\mathcal{H}(E_1 - E_2) + a\dot{E}_1,$$

we find a third background equation

$$E_3 = 3m_{Pl}^2 \left(\mathcal{H}^2 + \frac{\ddot{a}}{a} \right) - U_{,\phi} = 0. \tag{4.6}$$

By subtracting equation (4.4) from equation (4.5) we can find our first slow-roll parameter

$$\epsilon \equiv -\frac{\dot{\mathcal{H}}}{\mathcal{H}^2} = \frac{\ddot{\phi}}{2\mathcal{H}^2\phi} - \frac{\dot{\phi}}{2\mathcal{H}\phi}. \tag{4.7}$$

4.2 Expanding the Action to Second Order

Our goal in this chapter will be to set up what we need to eventually compute the bispectrum, for a selected $f(R)$ model chosen in Chapter 7, the 3-point correlation function as talked about in §2.8.2. However in order to do so we need to expand our action to third order.[1] On the way there, we will of course first need to expand the action to second order. We work with curvature perturbation $\mathcal{R}$. To expand the action we could have performed a split, like the ADM split [72]; however we have instead worked out a complete second order Ricci scalar from a completely general metric in Appendix A. In our case we choose to work in uniform field gauge, so that the components listed in the appendix reduce to,

$$\begin{aligned} \Phi &\rightarrow \Phi, \\ B_i &\rightarrow \partial_i \Psi, \\ C_{ij} &\rightarrow -\mathcal{R}\delta_{ij}. \end{aligned}$$

All of this will give us the new second order action,

$$\begin{aligned} S_2 = \int d^4x m_{Pl}^2 a \Bigg[&\frac{2\phi}{a}\dot{\mathcal{R}}\nabla^2\Psi - 3\phi\dot{\mathcal{R}}^2 - \frac{2\mathcal{H}\phi + \dot{\phi}}{a}\Phi\nabla^2\Psi - 2\phi\Phi\nabla^2\mathcal{R} \\ &+3(\mathcal{H}\phi + \dot{\phi})\Phi\dot{\mathcal{R}} - 3\mathcal{H}(\mathcal{H}\phi + \dot{\phi})\Phi^2 + \phi\partial_i\mathcal{R}\partial_i\mathcal{R} \Bigg]. \end{aligned} \tag{4.8}$$

We vary this action with respect to $\delta\Phi$ and find,

$$\nabla^2\Psi = -6a\mathcal{H}\frac{\mathcal{H}\phi + \dot{\phi}}{2\mathcal{H}\phi + \dot{\phi}}\Phi + 3a\dot{\mathcal{R}} - \frac{2a\phi}{2\mathcal{H}\phi + \dot{\phi}}\nabla^2\mathcal{R}, \tag{4.9}$$

and then we vary with respect to $\delta\Psi$ and find,

$$\Phi = \frac{2\phi}{2\mathcal{H}\phi + \dot{\phi}}\dot{\mathcal{R}}. \tag{4.10}$$

[1] We wish to calculate the bispectrum using second order perturbations, and an action always has to be evaluated one order above the desired perturbations.

Inserting equation (4.10) into equation (4.8), we will find a term $-2\phi\dot{\mathcal{R}}\nabla^2\mathcal{R}$ which we can integrate by parts so that,

$$S_2 = \int d^4x \frac{3m_{Pl}^2\phi\dot{\phi}}{(2\mathcal{H}\phi+\dot{\phi})^2}\left[a\dot{\mathcal{R}}^2 - c_s^2 a\partial_i\mathcal{R}\partial^i\mathcal{R}\right], \tag{4.11}$$

where c_s^2 is the speed of sound as earlier; we'll be working with $c_s^2 = 1$ during this chapter,[2] so this is the last time we'll see it. We can also rewrite equation (4.9) by introducing a dummy field χ,

$$\Psi = \frac{2a\Phi}{2\mathcal{H}\phi+\dot{\phi}}\mathcal{R} + \chi, \tag{4.12}$$

$$\nabla^2\chi = a\frac{3\dot{\phi}^2}{(2\mathcal{H}\phi+\dot{\phi})^2}\dot{\mathcal{R}}. \tag{4.13}$$

For the sake of keeping the expressions cleaner, let's define

$$Q \equiv \frac{3m_{Pl}^2\phi\dot{\phi}^2}{(2\mathcal{H}\phi+\dot{\phi})^2}. \tag{4.14}$$

The last thing we need for now, is to see how our field perturbations $\mathcal{R}$ evolve. We can find the equation of motion by using the Euler-Lagrange equations (2.6) with respect to $\mathcal{R}$ and using the constraint $\dfrac{\partial\mathcal{L}}{\partial\mathcal{R}} = 0$. We remember from the definition of the action $S = \int d^4x\mathcal{L}$ that the Lagrangian is hidden within equation (4.11),

$$\mathcal{L}_2 = Q\left[a\dot{\mathcal{R}}^2 - a\partial_i\mathcal{R}\partial^i\mathcal{R}\right] \Rightarrow \frac{d}{d\eta}\left(aQ\dot{\mathcal{R}}\right) - aQ\nabla^2\mathcal{R} = 0. \tag{4.15}$$

4.3 A Detour into Fourier Space

Continuing working in real space is going to be too inconvenient; we therefore perform transformation, so that

$$\mathcal{R}(\eta,\boldsymbol{x}) = \frac{1}{(2\pi)^3}\int d^3\boldsymbol{k}\mathcal{R}(\eta,\boldsymbol{k})e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \tag{4.16}$$

$$\mathcal{R}(\eta,\boldsymbol{k}) = u(\eta,\boldsymbol{k})a(\boldsymbol{k}) + u^*(\eta,-\boldsymbol{k})a^\dagger(-\boldsymbol{k}), \tag{4.17}$$

where we are using the annihilation and creation operators, obeying the commutators

$$\left[a(\boldsymbol{k}_1), a^\dagger(\boldsymbol{k}_2)\right] = (2\pi)^3\delta^{(3)}(\boldsymbol{k}_1 - \boldsymbol{k}_2), \quad [a(\boldsymbol{k}1), a(\boldsymbol{k}_2] = [a^\dagger(\boldsymbol{k}1), a^\dagger(\boldsymbol{k}_2] = 0. \tag{4.18}$$

Remember that switching to Fourier space boils down to letting $\frac{d}{dx} \to -i\boldsymbol{k}\cdot\mathbf{x}$, so that in our case $\nabla^2\mathcal{R} \to k^2\mathcal{R}$. Looking at just one of the u-modes in equation (4.17) and inserting it into equation (4.15), we see that u evolves as

$$\ddot{u} + \frac{\dot{(aQ)}}{aQ}\dot{\mathcal{R}} - k^2\mathcal{R} = 0, \tag{4.19}$$

[2] The speed of sound $c_s = 1$ for all $f(R)$ and scalar field models.

which we can solve to give us

$$u(\eta, \boldsymbol{k}) = \frac{i\mathcal{H}e^{-\boldsymbol{k}\eta}}{2\boldsymbol{k}^{3/2}\sqrt{Q}}\left(1 + i\boldsymbol{k}\eta\right). \tag{4.20}$$

At this point, we'll calculate the power spectrum, which we can find by the 2-point correlation function for the curvature perturbation,

$$\langle 0|\mathcal{R}(0,\boldsymbol{k})\mathcal{R}(0,\boldsymbol{k}')|0\rangle = \frac{2\pi^2}{\boldsymbol{k}^3}\mathcal{P}_{\mathcal{R}}(\boldsymbol{k})(2\pi)^3\delta^{(3)}(\boldsymbol{k}+\boldsymbol{k}') \tag{4.21}$$

$$\Rightarrow \mathcal{P}_{\mathcal{R}} = \frac{\mathcal{H}^2}{8\pi^2 a^2 Q} = \frac{\mathcal{H}^2(2\mathcal{H}\phi + \dot{\phi})^2}{24m_{Pl}^2\pi^2 a^2\phi\dot{\phi}^2}. \tag{4.22}$$

The spectral index is also of interest, which is defined by

$$n_s - 1 = \frac{d\ln\mathcal{P}_{\mathcal{R}}}{d\ln k}, \tag{4.23}$$

this is easier calculated when we realize that $\mathcal{R}$ will go constant when we approach the horizon, at $k < \mathcal{H}$, so that we only evaluate the power spectrum at $k = \mathcal{H}$. $\mathcal{H}$ vary slowly and that allow us to see that $d\ln k \approx d\ln a$[3]. This give us

$$n_{\mathcal{R}} - 1 = \frac{a}{\mathcal{P}_{\mathcal{R}}}\frac{d\mathcal{P}_{\mathcal{R}}}{da} = 2\frac{\dot{\mathcal{H}}}{\mathcal{H}^2} - \frac{\dot{\phi}}{\mathcal{H}\dot{\phi}} - \frac{\dot{\epsilon}_s}{\mathcal{H}\epsilon_s}, \tag{4.24}$$

where $\epsilon_s = \dfrac{\dot{\phi}}{2\mathcal{H}\phi} - \dfrac{\dot{\mathcal{H}}}{\mathcal{H}^2}$.

4.4 The Third Order Action

Similarly to how we got the second order action, equation (4.8), we could go forth to get a third order action. On the way there we would utilize equation (4.10) to eliminate all the Φ terms, introduce yet another dummy field, $\chi = m_{Pl}^2\frac{\phi}{a^2}\chi$ so that $\nabla^2\chi = Q\dot{\mathcal{R}}$, and use equation (4.9) to fully eliminate Ψ. Doing this would take quite a while, so we'll let Tsujikawa and De Felice do all the hacking and slashing for us in [2], so that the third order action goes as,

$$\begin{aligned} S_3 = \int d^4x \frac{3m_{Pl}^2 a\phi\dot{\phi}}{(2\mathcal{H}\phi + \dot{\phi})^4}\Big\{&(8\mathcal{H}\phi^2\ddot{\phi} + 4\phi\dot{\phi}\ddot{\phi} + 3\dot{\phi}^3 - 12\mathcal{H}\phi\dot{\phi}^2)\mathcal{R}(\partial\mathcal{R})^2 \\ &- a^2\phi\dot{\phi}(8\mathcal{H}\phi^2\ddot{\phi} + 4\phi\dot{\phi}\ddot{\phi} - 3\dot{\phi}^3 - 12\mathcal{H}\phi\dot{\phi}^2)\mathcal{R}\dot{\mathcal{R}}^2 \\ &- \frac{a^3\dot{\phi}^2}{2m_{Pl}^2}(16\mathcal{H}^2\phi^2 + 16\mathcal{H}\phi\dot{\phi} + \dot{\phi}^2)\dot{\mathcal{R}}(\partial_i\mathcal{R})(\partial_i\chi) \\ &+ \frac{a^2\dot{\phi}(2\mathcal{H}\phi + \dot{\phi})^2}{4m_{Pl}^4\phi^2}\nabla^2\mathcal{R}(\partial\chi)^2\Big\}. \end{aligned} \tag{4.25}$$

[3] $d\ln k = d\ln\mathcal{H} = \dfrac{1}{\mathcal{H}}\dfrac{d\mathcal{H}}{d\eta}d\eta$, using $\mathcal{H} = H_0(1 - H_0\eta)^{-1}$ as this is a de Sitter universe during inflation, we get $d\ln k = \mathcal{H}d\eta = d\ln a$.

4.5 Three-point Correlation Function and Bispectrum

Now let's set $S_3 = -\int dt\ H_{int}$, and compute the three-point correlation function by

$$\langle \mathcal{R}(\boldsymbol{k}_1)\mathcal{R}(\boldsymbol{k}_2)\mathcal{R}(\boldsymbol{k}_3)\rangle = -i\int_{-\infty}^{0} d\eta a \langle 0|[\mathcal{R}(0,\boldsymbol{k}_1)\mathcal{R}(0,\boldsymbol{k}_2)\mathcal{R}(0,\boldsymbol{k}_3), H_{int}(\eta)]|0\rangle, \quad (4.26)$$

keeping in mind that the $\mathcal{R}$'s in H_{int} are given in realspace and need to use the relation in equation (4.16) to get to Fourier space. We remember that the we find the bispectrum from $\langle \mathcal{R}(\boldsymbol{k}_1)\mathcal{R}(\boldsymbol{k}_2)\mathcal{R}(\boldsymbol{k}_3)\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3)\mathcal{B}_{\mathcal{R}}(k_1+k_2+k_3)$, where we get $(2\pi)^3\delta^{(3)}(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3)$ from the annihilation operators, leaving us with,

$$\mathcal{B}_{\mathcal{R}}(k_1,k_2,k_3) = \frac{(2\pi)^4}{(k_1k_2k_3)^3}\mathcal{A}_{\mathcal{R}}(k_1,k_2,k_3)\left[\mathcal{P}_{\mathcal{R}}(k_1)\mathcal{P}_{\mathcal{R}}(k_2) + 2\text{perms}\right], \quad (4.27)$$

where perms mean permutations and in this case would be 2perms $= \mathcal{P}_{\mathcal{R}}(k_1)\mathcal{P}_{\mathcal{R}}(k_3) + \mathcal{P}_{\mathcal{R}}(k_2)\mathcal{P}_{\mathcal{R}}(k_3)$. $\mathcal{A}_{\mathcal{R}}(k_1,k_2,k_3)$ is given, when using $K = (k_1+k_2+k_3)$, as

$$\begin{aligned}\mathcal{A}_{\mathcal{R}} = \frac{3\dot{\phi}^2}{(2\mathcal{H}\phi+\dot{\phi})^2}&\Bigg[\frac{1}{K}\sum_{i>j}^{3}k_i^2k_j^2 - \frac{1}{2K^2}\sum_{i\neq j}^{3}k_i^2k_j^3 \qquad (4.28)\\ &- \frac{12\mathcal{H}\phi\dot{\phi}^2 - 8\mathcal{H}\phi^2\ddot{\phi} - 4\phi\dot{\phi}\ddot{\phi} - 3\dot{\phi}^3}{24\dot{\phi}^3}\sum_{i=1}^{3}k_i^3\\ &- \frac{16\mathcal{H}^2\phi^2 + 16\mathcal{H}\phi\dot{\phi} + \dot{\phi}^2}{8(2\mathcal{H}\phi+\dot{\phi})^2}\left(\frac{1}{2}\sum_{i=1}^{3}k_i^3 - \frac{1}{4}\sum_{i\neq j}^{3}k_ik_j^2 - \frac{1}{K^2}\sum_{i\neq j}^{3}k_i^2k_j^3\right)\\ &+ \frac{3\dot{\phi}^2}{16(2\mathcal{H}\phi+\dot{\phi})^2}\frac{1}{K^2}\left(\sum_{i=1}^{3}k_i^5 + \frac{1}{2}\sum_{i\neq j}^{3}k_ik_j^4 - \frac{3}{2}\sum_{i\neq j}^{3}k_i^2k_j^3 - k_1k_2k_3\sum_{i>j}^{3}k_ik_j\right)\Bigg].\end{aligned}$$

4.5.1 The Non-Gaussianity Parameter

The magnitude of the non-Gaussianity, parametrized by the non-linearity parameter $f_{\rm NL}$, is given as [73]

$$f_{\rm NL} = \frac{5}{6}\frac{(k_1k_2k_3)^3}{k_1^3+k_2^3+k_3^3}\frac{\mathcal{B}_{\mathcal{R}}}{4\pi^4\mathcal{P}_{\mathcal{R}}^2} = \frac{10}{3}\frac{\mathcal{A}_{\mathcal{R}}}{k_1^3+k_2^3+k_3^3}, \quad (4.29)$$

where $\mathcal{P}_{\mathcal{R}}^2$ is a shorthand way of writing $\mathcal{P}_{\mathcal{R}}(k_1)\mathcal{P}_{\mathcal{R}}(k_2) + 2$perms. In order to calculate this number, an obvious question arises; what values do we choose for our various variables? Let us start by rewriting equation (4.28) with the help of the slow-roll parameters. First we rewrite equation (4.7) to the form,

$$2\epsilon_1 = -\epsilon_2 + \epsilon_2\epsilon_3, \quad (4.30)$$

where

$$\epsilon_1 = -\frac{\dot{\mathcal{H}}}{\mathcal{H}^2},\ \epsilon_2 = \frac{\dot{\phi}}{\mathcal{H}\phi},\ \epsilon_3 = \frac{\ddot{\phi}}{\mathcal{H}\dot{\phi}} = \frac{\ddot{\phi}}{\epsilon_2\mathcal{H}^2\phi}. \tag{4.31}$$

With this we get,

$$\begin{aligned}\mathcal{A}_{\mathcal{R}} = {} & D_1\left(\frac{1}{K}\sum_{i>j}^{3}k_i^2k_j^2 - \frac{1}{2K^2}\sum_{i\neq j}^{3}k_i^2k_j^3\right) - D_2\sum_{i=1}^{3}k_i^3 \\ & - D_3\left(\frac{1}{2}\sum_{i=1}^{3}k_i^3 - \frac{1}{4}\sum_{i\neq j}^{3}k_ik_j^2 - \frac{1}{K^2}\sum_{i\neq j}^{3}k_i^2k_j^3\right) \\ & + \frac{D_4}{K^2}\left(\sum_{i=1}^{3}k_i^5 + \frac{1}{2}\sum_{i\neq j}^{3}k_ik_j^4 - \frac{3}{2}\sum_{i\neq j}^{3}k_i^2k_j^3 - k_1k_2k_3\sum_{i>j}^{3}k_ik_j\right),\end{aligned} \tag{4.32}$$

where the coefficients are

$$D_1 = \frac{3\epsilon_2^2}{(2+\epsilon_2)^2}, \tag{4.33}$$

$$D_2 = \frac{12\epsilon_2 - 8\epsilon_3 - 4\epsilon_2\epsilon_3 - 3\epsilon_2^2}{8(2+\epsilon_2)^2}, \tag{4.34}$$

$$D_3 = \frac{3\epsilon_2^2(16+16\epsilon_2+\epsilon_2^2)}{8(2+\epsilon_2)^4}, \tag{4.35}$$

$$D_4 = \frac{9\epsilon_2^4}{16(2+\epsilon_2)^4}. \tag{4.36}$$

We will later see that we can relate the slow roll parameters ϵ_1, ϵ_2 and ϵ_3 to the number of e-foldings N.

4.5.2 The $\boldsymbol{k}$-configurations

One of the problems that arise at this point is the case of what values of k_1, k_2 and k_3 we should evaluate the different quantities at. In the literature cosmologists often simplify it down to the fact that the three ks should form a triangle,[4] and especially three forms of triangles dominate,

- **Equilateral configuration:** Where we set $k_1 = k_2 = k_3$.
- **Squeezed configuration:** Where we set $k_1 = k_2$, and $k_3 = 0$.
- **Colinear configuration:** Where we set $k_1 = k_2$, and $k_3 = 2k_1$.

[4]Letting the k's form a triangle can be interpreted as statistical isotropy.

One of our biggest questions is which of these configurations, if any, is the dominant one. The literature for $f(R)$ theories has a tendency to assume the equilateral one, so we will see if this is justified. The only thing left to do in order to calculate $\mathcal{A}_{\mathcal{R}}$, f_{NL} and $\mathcal{B}_{\mathcal{R}}$ is to assign values to the various slow-roll parameters; however in order to do so we need to specify a model first. We will pick a model and return to this discussion in Chapter 7.

Chapter 5

Gauge Issues between the Einstein and Jordan Frames

As described in §2.5.2, there is a practice of transforming from the frame one are working in, to another one where the equations are simpler or more numerically stable. However, it turns out that this holds a hidden danger, which, especially in numerical situations, can contaminate the results, if we don't make sure that we are working within a restricted set of gauges. The entirety of this chapter and its results has resulted in a paper published in Journal of Cosmology and Astroparticle Physics [1].

5.1 Transformations for a Perturbed Model

Considering the nature of the transformation for a perturbed model reveals an issue which to the best of our knowledge is as yet unappreciated by the literature. As mentioned, perturbed systems in relativity exhibit the gauge issue, choosing how to map fictitious background spacetime and the physical perturbed spacetime. In this chapter we consider the impact of this problem, and how one can resolve the resulting gauge ambiguities. We illustrate with a simple $f(R)$ model in a vacuum FLRW spacetime, but it should be emphasized that this issue will in principle occur in any perturbed spacetime and a wide range of extended theories of gravity.

While many authors working on perturbed spacetimes in modified gravity choose to employ "gauge-invariant" variables (for example, [74, 75]) or work in the Jordan frame (such as [76, 77, 78, 79, 80, 81, 82]), the analysis of gauge problems is necessary for three reasons. Firstly, there are authors who fix a gauge (such as [83, 53, 84, 85]), which is equally as valid. Secondly, gauge-invariant variables are themselves based on variables in a particular gauge [18]. The frequently-employed Bardeen potentials [86] are, for example, gauge-invariant generalizations of the potentials in conformal Newtonian gauge. If there is an issue with the choice of the "natural" gauge of a gauge-invariant perturbation, the perturbation itself cannot necessarily be trusted.

Numerical studies targeting the CMB and the matter power spectrum (such as [53, 48, 49, 50]) often employ modifications to Boltzmann codes such as CAMB [87], cmbeasy

[88], CLASS [89] or CosmoLib [90]. If there is an issue with the frame transformation and synchronous gauge, then the initial conditions for modifications of CAMB could be suspect, as could the final results even after being transformed back into the Jordan frame. Worse, if there is an issue the error is compounded: each transformation between frames will induce errors. Given that the use of CAMB (or similar codes) is of interest to us, the study of transformations of systems in synchronous gauge is forced upon us, despite its known shortcomings [18, 91].

The alternative formulation of $f(R)$ gravity employs the Palatini approach, where the metric and the connections are treated as independent objects. The nature of the transformation between the frames implies that the issues we highlight in this chapter are also relevant in the Palatini approach. Since the field equations in the Palatini approach are second order the usefulness of the transformation is somewhat lessened, but if a system is more easily evaluated in the Einstein frame then the potential ambiguities should still be considered.

The gauge problem is discussed and illustrated in §5.2. We finish the chapter with a summarization in §5.3 and a discussion of the implications in §5.4.

5.2 Perturbations and Gauge Issues in $f(R)$ Cosmology

5.2.1 Transforming Perturbations between Frames: Gauge Ambiguities

Remembering how transformations worked on the background level (2.28), let's look at how they transform perturbations. Applied to a linearly perturbed metric (2.85) and writing F and δF for the background and the perturbed quantity respectively, the conformal transformation between the frames is

$$\tilde{g}_{\mu\nu} = \tilde{g}^{(0)}_{\mu\nu} + \tilde{h}_{\mu\nu} = (F + \delta F)\left(g^{(0)}_{\mu\nu} + h_{\mu\nu}\right). \tag{5.1}$$

Assuming a flat FLRW background for illustration, all components of the metric imply

$$\tilde{a} = \sqrt{F}a \Rightarrow \tilde{\mathcal{H}} = \mathcal{H} + \frac{1}{2}\frac{\dot{F}}{F}. \tag{5.2}$$

The metric perturbation transforms as

$$\tilde{h}_{\mu\nu} = F h_{\mu\nu} + g^{(0)}_{\mu\nu}\delta F. \tag{5.3}$$

The perturbation can as we remember be expanded into scalar, vector and tensor modes [18] by

$$h_{\mu\nu}dx^\mu dx^\nu = \tag{5.4}$$

$$a^2(\eta)\left(-2\Phi d\eta^2 + (\partial_i B - S_i)\, d\eta dx^i - \left(2\Psi\delta_{ij} - 2\partial_i\partial_j E - 2\partial_{(i}F_{j)} - h^{(T)}_{ij}\right)dx^i dx^j\right),$$

with $\partial^i S_i = \partial^i F_j = \partial^i h^{(T)}_{ij} = \delta^{ij} h^{(T)}_{ij} = 0$. Applying the transformation leads ultimately to

$$\tilde{\Phi} = \Phi + \frac{1}{2}\frac{\delta F}{F}, \quad \tilde{\Psi} = \Psi - \frac{1}{2}\frac{\delta F}{F}, \tag{5.5}$$

with all other metric quantities invariant. The transformation then induces both a lapse Φ and a curvature Ψ regardless of the gauge chosen for $h_{\mu\nu}$. If for instance we employ uniform curvature gauge in the Jordan frame ($\Psi = E = 0$), giving us two scalar degrees of freedom Φ and B, then upon transformation into the Einstein frame we apparently have *three* scalar degrees of freedom, Φ, B and Ψ. Obviously these are not genuine degrees of freedom, being linear combinations of the two Jordan frame degrees of freedom. However, if the field equations are taken at face value, one should treat them as three. Erroneously employing the uniform curvature gauge field equations in the Einstein frame would in principle induce a gauge mode that would contaminate the results in the Einstein frame. Likewise, if we employed synchronous gauge in the Jordan frame, with $\Phi = B = 0$ and the degrees of freedom Ψ and E, upon transformation into the Einstein frame we would have three apparent degrees of freedom: Ψ, E and the redundant lapse Φ. Clearly if care is not taken the gauge is being tangled in the transformation between Jordan and Einstein frames – only gauges possessing both a lapse and a curvature, such as conformal Newtonian gauge, are unaffected.

We will now work out how all the various quantities transform. Let $u^\mu u^\nu T^{(M)}_{\mu\nu} = \rho_M(1+\delta_M)$ and $u^\mu_{(M)} = (1/a)(1-\Phi, \partial^i v_{(M)})$, and expand the scalar field $\tilde{\psi} = \kappa\tilde{\phi}$ as $\tilde{\psi} \to \tilde{\psi} + \delta\tilde{\psi}$. Then using the transformation of the stress energy tensor,

$$\tilde{T}_{\mu\nu} = \frac{T_{\mu\nu}}{F}, \tag{5.6}$$

which we expand to include perturbations with $F \to F + \delta F$,

$$\tilde{T}_{\mu\nu} = \frac{T_{\mu\nu}}{F + \delta F} = \frac{T_{\mu\nu}}{F}\left(1 - \frac{\delta F}{F}\right). \tag{5.7}$$

We can then quickly show, when using the perturbed stress-energy tensor in conformal Newtonian gauge,

$$T_{00} = a^2(\rho + \delta\rho + 2\Phi\rho), \; T_{0i} = -a^2(\rho + p)v_i \; T_{ij} = a^2\delta_{ij}(p + \delta p - 2\Psi p), \tag{5.8}$$

that

$$\tilde{T}_{00} = \frac{a^2\left(\rho + \delta\rho + 2\Phi\rho\right)}{F}\left(1 - \frac{\delta F}{F}\right) = \tilde{a}^2\left(\tilde{\rho} + \tilde{\delta\rho} + 2\tilde{\Phi}\tilde{\rho}\right) \tag{5.9}$$

$$\Rightarrow \tilde{\rho} + \tilde{\delta\rho} + 2\tilde{\Phi}\tilde{\rho} = \frac{1}{F^2}\left(\rho + \delta\rho + 2\Phi\rho - \frac{\delta F}{F}\rho\right). \tag{5.10}$$

When used alongside equation (5.5) demand that

$$\tilde{\rho} = \frac{\rho}{F^2}, \quad \tilde{\delta\rho} = \frac{\delta\rho}{F^2} - 2\frac{\rho\delta F}{F^3}, \tag{5.11}$$

and remembering the dimensionless density variable $\delta = \frac{\delta\rho}{\rho}$ we get,

$$\tilde{\delta} = \delta - 2\frac{\delta F}{F}. \tag{5.12}$$

With equation (5.11) and the Stefan-Boltzmann relation,

$$\rho \sim T^4,$$

we can see how the temperature transforms as well:

$$\tag{5.13}$$

Likewise,

$$\tilde{T}_{0i} = \frac{a^2(\rho+p)v_i}{F} = \frac{\tilde{a}^2(\rho+p)v_i}{F^2} = \tilde{a}^2(\tilde{\rho}+\tilde{p})\tilde{v}_i \tag{5.14}$$

$$\Rightarrow \tilde{v}_i = v_i \quad \text{and} \quad \tilde{p} = \frac{p}{F^2}. \tag{5.15}$$

Using the equation of state $p = w\rho$ we get,

$$\tilde{p} = \frac{p}{F^2} = w\frac{\rho}{F^2} = w\tilde{\rho} = \tilde{w}\tilde{\rho} \Rightarrow \tilde{w} = w. \tag{5.16}$$

Lastly,

$$\tilde{T}_{ij} = \frac{a^2\delta_{ij}\left(p + \delta p - 2\Psi p\right)}{F}\left(1 - \frac{\delta F}{F}\right) = \tilde{a}^2\left(\tilde{p} + \tilde{\delta p} - 2\tilde{\Psi}\tilde{p}\right) \tag{5.17}$$

$$\Rightarrow \tilde{p} + \tilde{\delta p} - 2\tilde{\Psi}\tilde{p} = \frac{1}{F^2}\left(p + \delta p - 2\Psi p - \frac{\delta F}{F}p\right), \tag{5.18}$$

which recovers what we previously have for the pressure, as well as giving us,

$$\tilde{\delta p} = \frac{\delta p}{F^2} - 2\frac{p\delta F}{F^3}. \tag{5.19}$$

Finally we want to see how the speed of sound transforms, we utilize the relation $\delta p = c_s^2\delta\rho$ so that,

$$\tilde{\delta p} = c_s^2\frac{\delta\rho}{F^2} - 2w\frac{\rho\delta F}{F^3} = c_s^2\left(\tilde{\delta\rho} + 2\frac{\rho\delta F}{F^3}\right) - 2w\frac{\rho\delta F}{F^3} \tag{5.20}$$

$$= c_s^2\tilde{\delta\rho} + 2(c_s^2 - w)\tilde{\rho}\frac{\delta F}{F}. \tag{5.21}$$

For the cases where $c_s^2 = w$[1] we see that the speed of sound is invariant, as were the equation of state and velocity under transformations.

[1] Which include all the cases we will look at in this thesis.

Finally, the scalar field is defined as

$$\tilde{\psi} = -\frac{1}{2Q}\ln F = -\frac{1}{2Q}\ln\left(F + \delta F\right) \Rightarrow \tilde{\psi} = -\frac{1}{2Q}\ln F, \quad \delta\tilde{\psi} = -\frac{1}{2Q}\frac{\delta F}{F}. \tag{5.22}$$

Summarizing, we have

$$\begin{array}{r|c}
\tilde{a} = \sqrt{F}a, & a = \tilde{a}\exp(Q\tilde{\psi}), \\
\tilde{\mathcal{H}} = \mathcal{H} + \dfrac{\dot{F}}{2F}, & \mathcal{H} = \tilde{\mathcal{H}} + Q\dot{\tilde{\psi}}, \\
\tilde{\rho} = \dfrac{\rho}{F^2}, & \rho = \tilde{\rho}\exp(-4Q\tilde{\psi}), \\
\tilde{p} = \dfrac{p}{F^2}, & p = \tilde{p}\exp(-4Q\tilde{\psi}), \\
\tilde{T} = \dfrac{T}{F^2}, & T = \tilde{T}\exp(-4Q\tilde{\psi}), \\
\tilde{\psi} = -\dfrac{1}{2Q}\ln F, & F = \exp(-2Q\tilde{\psi}), \\
\tilde{\Phi} = \Phi + \dfrac{\delta F}{2F}, & \Phi = \tilde{\Phi} + Q\delta\tilde{\psi}, \\
\tilde{\Psi} = \Psi - \dfrac{\delta F}{2F}, & \Psi = \tilde{\Psi} - Q\delta\tilde{\psi}, \\
\tilde{\delta} = \delta - \dfrac{2F}{F}, & \delta = \tilde{\delta} - 4Q\delta\tilde{\psi}, \\
\delta\tilde{p} = \dfrac{\delta p}{F^2} - 2\dfrac{p\delta F}{F^3}, & \delta p = \left(\delta\tilde{p} - 2Q\tilde{p}\delta\tilde{\psi}\right)\exp(-4Q\tilde{\psi}), \\
\tilde{v} = v, & v = \tilde{v}, \\
\delta\tilde{\psi} = -\dfrac{1}{2Q}\dfrac{\delta F}{F}, & \delta F = -2Q\delta\tilde{\psi}\exp(-2Q\tilde{\psi}).
\end{array} \tag{5.23}$$

As we see, the density perturbation also changes, implying that if we chose uniform density gauge in the Jordan frame we would no longer be in uniform density gauge following the conformal transformation.

Note that this issue only affects scalar perturbations and not vectors or tensors. It is also important to note that this is not unique to cosmological models; any system which is separated into a background metric plus perturbations will be at risk.

The cause of this is that the group associated with the conformal transformation is more tightly constrained than that of GR. The gauges that lie within this group are those with $\Phi \neq 0$, $\Psi \neq 0$ and $\delta\rho \neq 0$; synchronous, uniform curvature and uniform density gauges do not belong to this group, while conformal Newtonian and forms of co-moving gauges do. Practically, there are three straightforward approaches to dealing with the problem:

- One could choose to work directly with the additional redundant degree(s) of freedom in the Einstein frame, keeping those terms in the field equations.

- One could “refix” the gauge after a transformation. Transforming between the frames in the uniform curvature gauge induces a lapse; applying a gauge transformation into conformal Newtonian gauge or back into uniform curvature gauge will reabsorb these, explicitly leaving a system with two degrees of freedom.
- More physically, one could work in a gauge lying within the restricted group. The most obvious example is conformal Newtonian gauge, while other options would include a subset of the co-moving gauges with non-vanishing lapse and curvature.

It must be emphasized here that this is only an issue when the conformal transformation is applied – while in either frame, one may choose to work with any gauge, as normal. For instance, one should be able to transform in conformal Newtonian gauge into the Einstein frame, and then convert to uniform curvature gauge to undertake a calculation, before transforming back to conformal Newtonian gauge and transferring the result into the Jordan frame. As a result studies in Jordan frame that employ a gauge outside of the restricted class (such as [82]) remain entirely valid.

While employing a system with apparent redundant degrees of freedom might seem a bit odd, it can be easily justified. By the equivalence of the field equations (3.29) any solution valid in the Jordan frame is equally valid in the Einstein frame. A corollary is that, *as long as one employs the correct Einstein equations in the Einstein frame*, a Jordan frame solution will always be valid. However, these correct Einstein equations are not necessarily those that would be expected, and must additionally include the additional terms induced by the transformation. For example, the gauge-unfixed Hamiltonian constraint [18] is

$$3\tilde{\mathcal{H}}\left(\dot{\tilde{\Psi}}+\tilde{\mathcal{H}}\tilde{\Phi}\right)-\nabla^2\left(\tilde{\Psi}+\tilde{\mathcal{H}}\left(\dot{\tilde{E}}-\tilde{B}\right)\right)=-\frac{1}{2}\kappa^2\tilde{a}^2\delta\tilde{\rho}. \tag{5.24}$$

If we employ uniform curvature gauge in the Jordan frame with $\Psi = E = 0$ then we would in the Einstein frame naïvely expect to employ

$$3\tilde{\mathcal{H}}^2\tilde{\Phi}+\tilde{\mathcal{H}}\nabla^2\tilde{B}=-\frac{1}{2}\kappa^2\tilde{a}^2\delta\tilde{\rho}. \tag{5.25}$$

However, while we still have $\tilde{E} = 0$, here actually $\tilde{\Psi} \neq 0$. The correct version of the Hamiltonian constraint is then

$$3\tilde{\mathcal{H}}\left(\dot{\tilde{\Psi}}+\tilde{\mathcal{H}}\tilde{\Phi}\right)-\partial^i\partial_i\left(\tilde{\Psi}-\tilde{\mathcal{H}}\tilde{B}\right)=-\frac{1}{2}\kappa^2\tilde{a}^2\delta\tilde{\rho}. \tag{5.26}$$

The validity of this system is guaranteed by equation (3.29).

This might be unpalatable on practical grounds: a great advantage of working in the Einstein frame is to leverage existing codes which are written in a set gauge, and evolving the extra degree of freedom will involve additional coding and testing. Codes will also generally be more stable with two variables to evolve rather than three. One does, however, remain free to apply a gauge transformation into a more standard gauge. It is this which we refer to as “refixing”. The validity of the redundant system in the Einstein frame equally guarantees the validity of the refixed system. Since equation (3.29) guarantees the validity of the redundant system, the "refixed" system is equally valid given a well-defined gauge transformation. As such gauges such as uniform curvature and uniform density gauges can be seen as being clean when transforming between the Jordan and Einstein frames – and indeed are, so long as either the redundant system is evolved, or is reabsorbed following a gauge transformation. Failure to take one of these two steps will result in errors.

At this point it should be emphasized that CMB codes are commonly written in synchronous gauge [92, 93, 87, 89], as we will see later in Chapter 6. The transformation into synchronous gauge contains an arbitrary function of space [18]. We also note that one must work in conformal time instad of cosmic time in order to remove the ambiguity we discussed in §2.90, as in conformal time locking synchronous gauge to the velocity of cold dark matter will remove the ambiguity, this additional step must be taken if one is intending to use such a code in the Einstein frame. If one takes the Jordan frame to be the physical frame (in which the Hubble rate, matter densities, magnitude of perturbations are set), then the initial conditions must be set up in the Jordan frame and then transferred into the Einstein frame. To employ these in a Boltzmann code a further transformation into synchronous gauge is required *regardless of the gauge chosen in the Jordan frame*, and must be treated with the appropriate care.[2]

The final option is to work in a gauge lying in the restricted group. This group requires the existence of a lapse, a spatial curvature and matter perturbations. In the Jordan frame we have four metric and two matter scalar degree of freedoms, Φ, B, Ψ, E, $\delta\rho$ and v, of which we can remove two with gauge transformations. Of these, Φ, Ψ and $\delta\rho$ are non-zero in a gauge belonging to the restricted group. In vacuo, this limits us to conformal Newtonian gauge alone, while for systems with matter sources we have greater freedom and can also select co-moving gauges with $v = 0$ and either $E \neq 0$ or $B \neq 0$.

In the remainder of this chapter we illustrate this issue with a simple example system.

5.2.2 Is Flatness Preserved?

As a curiosity, we check to verify that flatness is preserved when we transform from one frame to another. This is technically imposed by the very nature of the transformations, but reaffirming this is easy, and worth doing just to be safe. Keeping equation (2.47), equation (3.11) (which is defined on a flat spacetime) and equation (2.71) in mind, we restate some quantities,

$$\tilde{\Omega}_m = \frac{\tilde{a}^2\kappa^2\tilde{\rho}_m}{3\tilde{\mathcal{H}}},\ \kappa^2\tilde{\rho}_\phi = \frac{1}{2\tilde{a}^2}\dot{\tilde{\psi}}^2 + \kappa^2\tilde{V} \Rightarrow \tilde{\Omega}_\phi = \frac{1}{3\tilde{\mathcal{H}}}\left(\frac{1}{2}\dot{\tilde{\Psi}}^2 + \tilde{a}^2\kappa^2\tilde{V}\right)$$

$$\dot{\tilde{\psi}} = -\frac{1}{2Q}\frac{\dot{F}}{F},\ \kappa^2\tilde{V} = \frac{RF - f}{2F^2},\ R = \frac{6}{a^2}\frac{\ddot{a}}{a}$$

[2] An interesting point that can be made here is that the conformal transformation does not preserve adiabaticity of initial conditions – that is, even if one sets adiabatic initial conditions in the Jordan frame, the introduction of an effective scalar field in the Einstein frame will induce a level of isocurvature, which should be taken into account. We show this in Chapter 6.

and remember all the transformations listed in the summarized equation set (5.23), we can set up,

$$
\begin{aligned}
3\tilde{\mathcal{H}}^2\left(\tilde{\Omega}_m+\tilde{\Omega}_\phi\right) &= \frac{a^2\kappa^2\rho_m}{F}+\frac{3}{4}\left(\frac{\dot{F}}{F}\right)^2+a^2\frac{RF-f}{F}\\
&= 3\mathcal{H}^2-3\frac{\ddot{a}}{a}+\frac{a^2}{2}\frac{f}{F}+3\mathcal{H}\frac{\dot{F}}{F}+\frac{3}{4}\left(\frac{\dot{F}}{F}\right)^2+3\frac{\ddot{a}}{a}-\frac{a^2}{2}\frac{f}{F}\\
&= 3\left(\mathcal{H}^2+\mathcal{H}\frac{\dot{F}}{F}+\frac{1}{4}\left(\frac{\dot{F}}{F}\right)^2\right)\\
&= 3\left(\mathcal{H}+\frac{1}{2}\frac{\dot{F}}{F}\right)^2=3\tilde{\mathcal{H}}^2.
\end{aligned}
$$

As we see, $\tilde{\Omega}_m+\tilde{\Omega}_\phi=1$ is implied by this calculation. Now we continue on to the example system.

5.2.3 Gauge Issues in Vacuum Polynomial Gravity

In this section we focus on polynomial gravity, with

$$f(R)=\alpha R^n \;\Rightarrow F=\alpha n R^{n-1}. \tag{5.27}$$

The background cosmology of this theory has been considered in detail in [47]. These authors found the exact background solution both in vacuum and in the presence of matter fields,

$$a\propto t^{(1-n)(2n-1)/(n-2)}. \tag{5.28}$$

The exponent diverges when $n\to 2$, suggesting that it is a particularly interesting case.

The situation is clearer in the Einstein frame. The scalar field potential (3.20) becomes

$$\kappa^2\tilde{V}(\tilde{\phi})=\frac{1}{2\alpha^{1/(n-1)}}\frac{n-1}{n^{n/(n-1)}}\exp\left(2\frac{n-2}{n-1}Q\kappa\tilde{\phi}\right), \tag{5.29}$$

which is constant for $n=2$. For particular initial data or at late times we would then expect $(d\tilde{\phi}/dt)^2\ll\tilde{V}(\tilde{\phi})$, and the spacetime in the Einstein frame will become de Sitter. For a field with $\dot{\tilde{\psi}}=0$, equation (5.2) implies that the scale factor retains its character – an exponential expansion in the Einstein frame will map onto an exponential expansion in the Jordan frame. When $n=2$, the solution in the Jordan frame is therefore de Sitter. This has been noted before in [94], where $n=2$ is shown to correspond to $w_{\text{eff}}=-1$, and in [47] where it is stated that $\alpha\propto(n-2)=0$ corresponds to de Sitter space.

We take $n=2$ and for simplicity we work on superhorizon scales in vacuum; this simplifies the treatment of the perturbations considerably.

Background

Inserting the test model equation (5.27) into the Einstein field equations in the Jordan frame equation (3.11) give us

$$3\left(\frac{\dot{a}}{a}\right)^2+\frac{a^2}{4}R-3\frac{\ddot{a}}{a}+3\frac{\dot{a}}{a}\frac{\dot{R}}{R}=0,\quad \frac{\ddot{a}}{a}+\left(\frac{\dot{a}}{a}\right)^2-\frac{\ddot{R}}{R}-\frac{\dot{a}}{a}\frac{\dot{R}}{R}-\frac{a^2}{4}R=0. \tag{5.30}$$

The solution (5.28) is in coordinate time. A solution for this system in conformal time is

$$a(\eta)=(1+H_0(\eta_0-\eta))^{-1}\Rightarrow F=24\alpha H_0^2, \tag{5.31}$$

where $\mathcal{H}=aH_0$ and we have normalized such that $a(\eta_0)=1$. Remember, we opt to write the scalar field in units of κ, $\tilde{\psi}=\kappa\tilde{\phi}$, the Friedmann and continuity equations in the Einstein frame are as we remember,

$$3\left(\frac{\dot{\tilde{a}}}{\tilde{a}}\right)^2=\tilde{a}^2\kappa^2\tilde{\rho}_\phi,\quad \dot{\tilde{\rho}}_\phi+3\tilde{\mathcal{H}}\left(\tilde{\rho}_\phi+\tilde{p}_\phi\right)=0, \tag{5.32}$$

where

$$\tilde{\rho}_\phi=\frac{1}{2\tilde{a}^2\kappa^2}\dot{\tilde{\psi}}^2+\tilde{V}(\tilde{\phi}),\quad \tilde{p}_\phi=\tilde{\rho}_\phi-2\tilde{V}(\tilde{\phi}),\quad \kappa^2\tilde{V}(\tilde{\phi})=\frac{1}{8\alpha}. \tag{5.33}$$

The solution (5.31) transformed into the Einstein frame is

$$\tilde{a}=\frac{\sqrt{24\alpha}H_0}{1+H_0(\eta_0-\eta)},\quad \tilde{\psi}=-\frac{1}{2Q}\ln\left(24\alpha H_0^2\right),\quad \tilde{w}_\phi=-1. \tag{5.34}$$

The effective scalar field in the Einstein frame is frozen on a constant potential; as in the Jordan frame, this is de Sitter space.

This solution corresponds to the case where $\psi\equiv$ const., which reduces the effective scalar field energy and pressure to constants. The system in the Einstein frame admits a more general case, corresponding to a field which is initially rolling in the potential before slowing through Hubble friction. By inserting equation (5.33) into equation (5.32) we find a continuity equation for the scalar field, which can be written as

$$\frac{\partial}{\partial\tilde{a}}\left(\tilde{a}^6\kappa^2\tilde{\rho}_\phi\right)=\frac{3\tilde{a}^5}{4\alpha}, \tag{5.35}$$

which can be solved to yield

$$\kappa^2\tilde{\rho}_\phi=\frac{A}{\tilde{a}^6}+\frac{1}{8\alpha}. \tag{5.36}$$

If the initial conditions are tuned such that $A=0$, or when $\tilde{a}\gg 1$, then $\psi\equiv$ const and this solution is the de Sitter limit found above. There is also a “dynamic limit” where the density decays rapidly with time, $\kappa^2\tilde{\rho}_\phi = A/\tilde{a}^6$, with $\tilde{a} = (2\sqrt{A/3}(\eta_0 - \eta))^{1/2}$, which holds when $\tilde{a} \ll (8\alpha A)^{1/6}$. An implicit general solution for a is

$$\eta = \frac{4}{9}\left(\frac{16\alpha^2}{A}\right)^{1/6} \frac{\sqrt{3}\pi^2}{\left(\Gamma(2/3)\right)^3} - \frac{\sqrt{24\alpha}}{\tilde{a}}\, {}_2\mathcal{F}_1\left(\frac{1}{6}, \frac{1}{2}; \frac{7}{6}; -\frac{8A\alpha}{\tilde{a}^6}\right), \tag{5.37}$$

where ${}_2\mathcal{F}_1(a;b;x)$ is a regular hypergeometric function. In the limit $a \to \infty$ this tends to de Sitter space[3]. For our purposes it is thankfully sufficient to work in the de Sitter limit.

Linear Perturbations in the Restricted Group

In this section we find solutions for the perturbed vacuum spacetime in conformal Newtonian gauge and demonstrate that the system is trivially valid in the Einstein frame in both the conformal Newtonian and the uniform curvature gauges. Conformal Newtonian gauge lies in the restricted class of gauges, while uniform curvature gauge does not. The restricted gauge group consists of the usual gauge group in relativity with the additional conditions $\Phi \neq 0$ and $\Psi \neq 0$. The uniform density and uniform field gauges are other examples of gauges satisfying these conditions. On large scales where spatial derivatives can be neglected the vacuum perturbation equations [53], where we write $\delta F = \frac{\partial F}{\partial R}\delta R$, are

$$F\left(\Phi - \Psi\right) + \frac{\partial F}{\partial R}\delta R = 0,$$
$$6\mathcal{H}F\left(\dot{\Psi} + \mathcal{H}\Phi\right) + 3\frac{\partial F}{\partial R}\dot{\mathcal{H}}\delta R - 3\mathcal{H}\frac{\partial}{\partial \eta}\left(\frac{\partial F}{\partial R}\right)\delta R - 3\mathcal{H}\frac{\partial F}{\partial R}\delta\dot{R} + 3\dot{F}\left(2\mathcal{H}\Phi + \dot{\Psi}\right) = 0, \tag{5.38}$$

where it is understood that F and R are background quantities. Inserting our model with $F = 2\alpha R$ and using

$$\delta R = -\frac{6}{a^2}\left(2\frac{\ddot{a}}{a}\Phi + \mathcal{H}\dot{\Phi} + 3\mathcal{H}\dot{\Psi} + \ddot{\Psi}\right), \tag{5.39}$$

one can find that

$$\Psi = \Psi_1 + \frac{\Psi_2}{a} + \frac{\Psi_3}{a^3}, \quad \Phi = \frac{\Psi_2}{a} - \frac{\Psi_3}{a^3} - \Psi_1, \tag{5.40}$$

is a general solution. Therefore

$$\frac{\delta F}{F} = 2\left(\Psi_1 + \frac{\Psi_3}{a^3}\right). \tag{5.41}$$

[3]Note that this solution is not normalized such that $a(\eta_0) = 1$.

This solution is transformed to the Einstein frame using the transformations defined in (5.23), giving $\tilde{\Phi} = \tilde{\Psi}$ and

$$\tilde{\Phi} = \frac{\Psi_2}{a} = \frac{\sqrt{24\alpha} H_0 \Psi_2}{\tilde{a}}, \quad \delta\psi = -\frac{1}{Q}\left(\Psi_1 + \frac{(24\alpha)^{3/2} H_0^3 \Psi_3}{\tilde{a}^3}\right). \tag{5.42}$$

Then $\dot{\psi} = 0$ at a background level, implying $8\alpha\kappa^2\tilde{\rho}_\phi = 1$ and $\delta\tilde{\rho}_\phi = \delta\tilde{p}_\phi = 0$. The Newtonian potentials are equal, as should be expected since in the Einstein frame, unlike the Jordan frame, the anisotropic stress vanishes. The Klein-Gordon equation, Hamiltonian constraint and shear evolution equations [18] in this frame are,

$$\tilde{\mathcal{H}}\left(\dot{\tilde{\Phi}} + \tilde{\mathcal{H}}\tilde{\Phi}\right) = 0, \tag{5.43}$$

$$\tilde{\Phi} = \tilde{\Psi}, \tag{5.44}$$

$$\delta\ddot{\tilde{\psi}} + 2\tilde{\mathcal{H}}\delta\dot{\tilde{\psi}} = 0, \tag{5.45}$$

which are clearly satisfied. This illustrates the expected equivalence between the frames: a system perturbed in conformal Newtonian gauge can be evolved in either the Jordan or the Einstein frames, to yield a consistent result in the Jordan frame. The same holds for any gauge that lies within the restricted group.

A scalar quantity transforms under a gauge transformation $\xi^\mu = (\alpha, \partial^i\beta)$ as $\delta A_{\mathrm{F}} = \delta A + \dot{A}\alpha$ [18], and so is gauge-invariant at linear order if it is constant on the background. As a result, the field perturbation is gauge-invariant because $\dot{\tilde{\psi}} = 0$, and will therefore always satisfy its equation of motion. The transformation from conformal Newtonian into uniform curvature gauge, defined by choosing $\Psi_{\mathrm{F}} = E_{\mathrm{F}} = 0$ [18], is

$$\tilde{\Phi}_{\mathrm{F}} = \tilde{\Phi} + \tilde{\Psi} + \frac{\partial}{\partial\eta}\left(\frac{\tilde{\Psi}}{\tilde{\mathcal{H}}}\right), \quad \tilde{B}_{\mathrm{F}} = -\frac{\tilde{\Psi}}{\tilde{\mathcal{H}}}, \tag{5.46}$$

where a subscript F denotes uniform curvature gauge. Uniform curvature gauge was used in, for example, [95]. The lapse and shift in uniform curvature gauge are then

$$\tilde{\Phi}_{\mathrm{F}} = 0, \quad \tilde{B}_{\mathrm{F}} = -\frac{24\alpha H_0^2}{\tilde{a}^2}\Psi_2. \tag{5.47}$$

The Hamiltonian constraint and shear evolution become

$$3\tilde{\mathcal{H}}^2\tilde{\Phi}_{\mathrm{F}} = 0, \quad \dot{\tilde{B}}_F + 2\tilde{\mathcal{H}}\tilde{B}_F = 0, \tag{5.48}$$

which are clearly satisfied.

Refixing a Gauge

Consider the system in the uniform curvature gauge in the Jordan frame. Transforming the Jordan frame solutions (5.40) into uniform curvature gauge gives

$$\Phi_{\mathrm{F}} = -\Psi_1 - 4\frac{\Psi_3}{a^3}, \quad B_{\mathrm{F}} = -\frac{1}{aH_0}\left(\Psi_1 + \frac{\Psi_2}{a} + \frac{\Psi_3}{a^3}\right). \tag{5.49}$$

Since the background Ricci scalar is constant, the perturbed Ricci scalar is gauge-invariant and $\delta F/F$ is given by equation (5.41). Transforming into the Einstein frame gives

$$\begin{aligned}\tilde{\Phi}_{\mathrm{F},2} &= -3(24\alpha)^{3/2}H_0^3\frac{\Psi_3}{\tilde{a}^3}, \quad \tilde{\Psi}_{\mathrm{F},2} = -\Psi_1 - (24\alpha)^{3/2}H_0^3\frac{\Psi_3}{\tilde{a}^3}, \\ \tilde{B}_{\mathrm{F},2} &= -\frac{\sqrt{24\alpha}}{\tilde{a}}\left(\Psi_1 + \sqrt{24\alpha}H_0\frac{\Psi_2}{\tilde{a}} + (24\alpha)^{3/2}H_0^3\frac{\Psi_3}{\tilde{a}^3}\right),\end{aligned} \tag{5.50}$$

which evidently differ from (5.47). In particular, since the lapse is non-vanishing the Hamiltonian constraint is satisfied only if $\Psi_1 = 0$, while the stress evolution equation is only valid if $\Psi_1 = \Psi_3 = 0$ – neither of which are acceptable.

Consider a model in units where $\alpha = H_0 = 1$, and set the initial conditions $\Psi = 1$, $\dot{\Psi} = 0$, $\ddot{\Psi} = 1/2$ in the Jordan frame at $a = 1$. Then we find

$$\Psi_1 = \frac{7}{6}, \quad \Psi_2 = -\frac{1}{4}, \quad \Psi_3 = \frac{1}{12}. \tag{5.51}$$

Transferring into the Einstein frame, we find that $a = 1$ corresponds to $\tilde{a} = \sqrt{24}$. On this time-slice equation (5.50) implies that $\tilde{B}_{F,2}(\tilde{a} = \sqrt{24}) = -1$. Equations (5.48) then implies that

$$\tilde{B}_{F,2} = -\frac{24}{\tilde{a}^2} \tag{5.52}$$

is the "solution" in the Einstein frame. However, equation (5.47) shows that

$$\tilde{B}_F = -\frac{24}{\tilde{a}^2}\Psi_2 = \frac{6}{\tilde{a}^2}. \tag{5.53}$$

The difference is of the same order of magnitude as the perturbation itself. Worse, if we performed the transformation on a different time-slice we would obtain different results. Even worse, transferring the lapse gives $\tilde{\Phi}_{\mathrm{F},2}(\tilde{a} = \sqrt{24}) = -1/4$ on the initial hypersurface but equations (5.48) enforce $\tilde{\Phi}_{\mathrm{F}} = 0$ at all other times.

This illustrates the main result of this chapter and our paper [1]: if you naïvely transfer a system in an unsafe gauge between the Jordan and Einstein frames, you will inevitably introduce errors of the same order of magnitude as the perturbations themselves.

In the previous section we argued two approaches to dealing with this: refixing the gauge, and employing a redundant set of field equations. Consider first refixing the gauge to uniform curvature gauge by reabsorbing the spatial curvature with the general transformations

$$\tilde{\Phi}_{\mathrm{RF,F}} = \tilde{\Phi}_{\mathrm{F},2} + \tilde{\Psi}_{\mathrm{F},2} + \frac{\partial}{\partial\eta}\left(\frac{\tilde{\Psi}_{\mathrm{F},2}}{\tilde{\mathcal{H}}}\right) = 0, \quad \tilde{B}_{\mathrm{RF,F}} = \tilde{B}_{\mathrm{F},2} - \frac{\tilde{\Psi}_{\mathrm{F},2}}{\tilde{\mathcal{H}}} = -\frac{24\alpha H_0\Psi_2}{\tilde{a}^2} \tag{5.54}$$

in agreement with (5.47). Likewise, refixing to conformal Newtonian gauge,

$$\tilde{\Phi}_{\mathrm{RF,N}} = \tilde{\Phi}_{\mathrm{F},2} + \dot{\tilde{B}}_{\mathrm{F},2} + \tilde{\mathcal{H}}\tilde{B}_{\mathrm{F},2} = \sqrt{24\alpha}H_0\frac{\Psi_2}{\tilde{a}}, \quad \tilde{\Psi}_{\mathrm{RF,N}} = \tilde{\Psi}_{\mathrm{F},2} - \tilde{\mathcal{H}}\tilde{B}_{\mathrm{F},2} = \tilde{\Phi}_{\mathrm{RF,N}} \tag{5.55}$$

in agreement with (5.42). These illustrate the validity of refixing the gauge to reabsorb the unexpected degree of freedom.

We can also consider the unfixed system in the Einstein frame. We have three scalar degrees of freedom: $\tilde{\Phi}_{\mathrm{F}}$, $\tilde{\Psi}_{\mathrm{F}}$ and $\tilde{B}_{\mathrm{F}}$. Retaining these three variables, the vacuum field equations on large scales [18] are

$$3\tilde{\mathcal{H}}\left(\dot{\tilde{\Psi}}_{\mathrm{F},2} + \tilde{\mathcal{H}}\tilde{\Phi}_{\mathrm{F},2}\right) = 0, \tag{5.56}$$

$$\dot{\tilde{B}}_{\mathrm{F},2} + 2\tilde{\mathcal{H}}\tilde{B}_{\mathrm{F},2} + \tilde{\Phi}_{\mathrm{F},2} - \tilde{\Psi}_{\mathrm{F},2} = 0, \tag{5.57}$$

$$\ddot{\tilde{\Psi}}_{\mathrm{F},2} + 2\tilde{\mathcal{H}}\dot{\tilde{\Psi}}_{\mathrm{F},2} + \tilde{\mathcal{H}}\dot{\tilde{\Phi}}_{\mathrm{F},2} + \left(2\dot{\tilde{\mathcal{H}}} + \tilde{\mathcal{H}}^2\right)\tilde{\Phi}_{\mathrm{F},2} = 0. \tag{5.58}$$

These field equations are also clearly satisfied by equations (5.50).

5.3 Summarizing

In this chapter we have discussed a technical subtlety of the conformal transformation between the Jordan and Einstein frames that to the best of our knowledge has not been highlighted before: naïvely transferring a perturbed system between the frames tangles your choice of gauge. It should be emphasized that this effect is *calculational*, not physical, and that if sufficient care has been taken no previous results are changed by this. It is also extremely important to note that this issue is not restricted to $f(R)$ gravity or to the study of cosmological perturbations, and that it potentially arises whenever a perturbed system is conformally transformed regardless of the background metric or the model of gravity. $f(R)$ theory and vacuum cosmology provide a useful, straightforward illustration of this. While we have concretely demonstrated the issue only for this vacuum $f(R)$ system, in principle it arises generically, although demonstrating this explicitly is beyond the scope of this thesis.

The properties of the conformal transformation restrict us to a particular set of gauges which we refer to as the "restricted group": gauges that possess a lapse, a spatial curvature, and a density perturbation. This restriction only applies when the transformation is performed. At all other times one is free to work in any convenient gauge. However, we additionally argued that there are alternatives to working in the restricted group – one can instead choose to "refix" the gauge, or to evolve the system using the redundant Einstein field equations.

We have illustrated our arguments with a simple vacuum system, showing that there are no ambiguities introduced by equations (5.23), so long as one takes care to refix the gauge, to work with a redundant set of field equations, or to ensure one works in a gauge that lies in the restricted group. If this is not done and the results of a transformation from a gauge outside the restricted group are interpreted as if they themselves lie in that gauge, the system will be inaccurately specified.

5.4 Implications

Perhaps the most important situation where this issue will arise is in the treatment of initial conditions. For instance, Boltzmann codes are frequently [92, 93, 87, 89] written in synchronous gauge, which lies outside of the restricted group. Interpreting the Jordan frame as the physical frame, the initial conditions must be set in the Jordan frame. It seems natural to set them in the synchronous gauge and transfer these initial conditions to the Einstein frame. However, regardless of the gauge chosen, the transformation induces a lapse function which must be reabsorbed if the results of the calculation are to make any sense. This itself introduces an additional problem: the transformation to synchronous gauge is not fully specified, and introduces an arbitrary function of the curvature which must itself be removed with care. The alternative is to include the redundant degrees of freedom in the Boltzmann codes, which requires additional effort. A careless study without attention to these issues would either leave the system with the spurious lapse, or risk introducing a gauge mode. Some Boltzmann codes [92, 88, 89] include modules written in conformal Newtonian gauge, which lies within the restricted group, and studies of extended gravity that employ these codes remain consistent. However the study of synchronous gauge is forced upon us by CAMB, which given the widespread use of Fortran in cosmology, its large codebase and the extensive testing it has undergone, is the dominant Boltzmann code. Similar arguments apply to the initial conditions employed in n-body simulations of modified gravity performed in the Einstein frame.

The other time at which the gauge ambiguity becomes important is at the end of a calculation. Taking the Jordan frame to be physical, the results of a simulation in the Einstein frame must be transformed back. Given that calculations are frequently performed in synchronous gauge then one must either transform into a safer gauge before performing the conformal transformation, or deal with the redundant system in the Jordan frame. Otherwise one runs a serious risk of contamination. At this stage it seems easier to refix the gauge in the Jordan frame to a fully-specified gauge (such as conformal Newtonian or uniform curvature), or to leave the system unspecified. So long as one does so consistently, observables will not be affected, since gauge transformations cannot change an observation.

It is interesting to note that the lensing potential $\Phi + \Psi$ is uncontaminated by the transformation. As such, if one wishes to calculate the weak lensing signal on a constant-time hypersurface, this can be achieved transforming from the Jordan frame into the Einstein frame in any gauge and not worrying about refixing the system [52]. For a static (or quasi-static) system, this will be a good approximation. However, carelessly evolving the system without care will in principle introduce errors, so that the frame invariance does not imply such a straightforward estimate of the integrated Sachs-Wolfe effect [3].

Chapter 6

Modifying CAMB

In the previous chapter we showed how the transformation between Jordan and Einstein frames can induse errors if we're not working within a restricted set of gauges, of which conformal Newtonian gauge is the preferred choice. Boltzmann codes are much used in the field of cosmology to study the CMB, and existing Boltzmann codes are extensively developed and contain a wealth of physics which we can leverage with minimal modification. With this in mind we wish to modify a full-featured Boltzmann code in the Einstein frame, which could be used with minimal modifications to study arbitrary modified gravities that admit an Einstein frame representation. Steps towards this have been done before [96, 97, 53], but none of these are tailored to safeguard the problems above. Sections of this chapter are based on an ongoing research project.

6.1 Why CAMB?

The original intent was to produce my own selfcontained Boltzmann code, however as progress was made it soon became clear that this task would be too big to finish within the timeframe of this thesis. Therefore the choice was easy, we would rather modify an existing code, notably CAMB. We have decided to modify CAMB not only to safeguard against the issues found in Chapter 5, but also to generalize it to allow any modified gravity that has an Einstein frame representation. But why did we choose CAMB? Let us take a look at our choices.

1. COSMICS: The grandfather of Boltzmann codes, it was written in Fortran 77 by Bertschinger [92] and works in both the conformal Newtonian and the synchronous gauges. COSMICS has long been dead, superceded by CMBFast which is orders of magnitude quicker. No-one would do research on COSMICS without a lot of modification to add improvements already in modern codes.

2. CMBFast: The father of Boltzmann codes, CMBFast is a line-of-sight CMB integrator that uses the synchronous gauge side of COSMICS as its core. Programmed in Fortran 77 by Seljak and Zaldariagga [93], CMBFast has also long been dead, superceded by CAMB which has superior data-exchange facilities, support for

palatalization, bug fixes etc. CMBFast could be used, but the decoupling physics in particular are very out of date and it is generally much less stable than its successors.

3. cmbeasy: The younger brother of CAMB, cmbeasy is a C++ port of CMBFast originally by Doran [88] and then maintained by Robbers. It hasn't been updated for a few years, although we believe it is still in private development. Despite its inheritance from CMBFast, cmbeasy now employs a gauge-invariant formalism based on the Bardeen potentials [86] and is therefore effectively in conformal Newtonian gauge, and has an independent core to CAMB. Little used, partly because it is programmed in C++. cmbeasy interfaces tightly with its own parameter estimation code, AnalyzeThis! [98].

4. CAMB: The king of Boltzmann codes, CAMB started as a Fortran 90 port of CMBFast. Re-derived and rewritten in the gauge-invariant and covariant approach to cosmology, but locked to zero-CDM-acceleration frame, which is equivalent to synchronous gauge, for all practical purposes we can treat CAMB as being another synchronous gauge code. CAMB is used by the vast majority of papers on linear cosmology. Plenty of modifications already exist: MGCAMB [48], IsItGR? [51] and others [99, 100]. It also interfaces nicely with CosmoMC [101] which is used by the vast majority of parameter estimation studies.

5. CLASS: While CAMB in particular is extensively tested, it is not very user-friendly, particularly to modify. To this end Lesgourgues programmed CLASS in C [89]. Unlike CAMB, CLASS integrates the background independently from the perturbations, whereas CAMB integrates it whenever it integrates a perturbed variable, which is wasteful. CLASS is too new to know what acceptance it will have, but such is likely to be limited by the fact it is coded in C. CLASS was initially released in synchronous gauge, which remains better tested, although a conformal Newtonian gauge module was released soon after.

6. COSMOLib: Programmed with many of the same aims as CLASS, predominantly in Fortran 90 but with some calls to routines written in C. COSMOLib is far too new to know what impact it will have, and boasts tight integration with its own MCMC routines for parameter estimation. The greatest benefit of CosmoLib is that it was programmed from the start in conformal Newtonian gauge and its conformal Newtonian module has been tested more extensively than that of CLASS. Being written in F90 is also a bonus, as it is more familiar to academics than C or C++.

Since COSMICS and CMBFast have long been dead, and the development of cmbeasy is on hold, the realistic choices are between CAMB, CLASS and CosmoLib. We choose to work with CAMB mainly because it is the dominant code and contains the greatest wealth of physics. While CosmoLib also looks extremely interesting – being programmed from scratch in the familiar Fortran 90 and in conformal Newtonian gauge could prove extremely useful – it contains much less physics than CAMB. CLASS is a tightly-programmed code which is extremely pleasant to use; however, our familiarity with C is not developed enough to modify it reliably.

6.2 Structure of CAMB

Here follows a brief overview of CAMB's structure.

- Start by inputting the density parameters Ω_{x0}, Hubble constant $\mathcal{H}_0$, equation of state w_0 etc, the CMB temperature $T_{\rm CMB}$ and various other variables.
- Integrate the perturbed quantities Φ, Ψ, δ_x, v_x etc. For each of these CAMB integrates the background.
- Calls the Recfast module calculating the decoupling physics, while also recovering the background quantities from CAMB.
- Construction of the various sources, represented by the source function $s_l(k,\eta)$.
- Once perturbations are finished evolving, construct the angular power spectrum C_l, brightness function Δ_{Tl} and matter power spectrum $|\delta_m|^2$.
- Output C_l and $|\delta_m|^2$ to file.

6.3 Modifications

Although our motivation comes from modified gravities, there is a second useful consequence of our modification of CAMB: the background dependence has been stripped from the code, in the manner of very recent codes such as CLASS and CosmoLib, vastly improving the functionality. The code we are developing contains modules allowing standard ΛCDM, wCDM with constant or varying w and arbitrary speeds of sound, single-field quintessence models, coupled quintessence models, and simple models of extended gravity. It is straightforward to add in further models, and changes to the background propagate automatically through the code.

Note that we assume that FLRW is a solution to our theory, that the matter fluids are perfect, and that a conformal transformation can be made into an Einstein frame. The form of theory is otherwise unspecified, although it is an implicit assumption that the Einstein frame will possess only one scalar field, which is related to our Jordan frame possessing only one additional degree of freedom ($F(R)$, or ϕ in an $f(R)$ or scalar-tensor model). The details of the model in the Jordan and Einstein frames are added as single functions in a module visible to the rest of the code.

The outline of our code goes as this: We introduce the initial conditions in the conformal Newtonian gauge, so that we can immediately transfer to the Einstein frame without worrying about any new degrees of freedom. Once in the Einstein frame, we refix the initial conditions to synchronous gauge, for so to continue the evolution using synchronous gauge evolution equations (2.114)-(2.117), just as vanilla CAMB. At the very end of this evolution, we would perform a new transformation into conformal Newtonian Gauge, before swapping back to the Jordan frame. However this last step might be redundant if all we want is the CMB powerspectrum, which can be directly constructed in the Einstein frame. We will show that when we transform between the frames we will introduce isocurvature[1] in the Einstein frame.

If $f(R) \approx R$ when we start the code, then we can use modifications of the standard Ma and Bertschinger initial conditions [21]; otherwise we need to re-derive them. These standard initial conditions will require a long-lasting radiation epoch. First and foremost we find conditions from M&B that hold, and derive them with first order modifications.

The Einstein frame physics from radiation domination all the way through to the current epoch remains unchanged in form from GR and the code will need minimal modifications. When we get to the point of computing the CMB and the matter power spectrum, we will store the brightness functions to disc, so they can be used with higher order statistics[2].

We choose to take the Jordan frame as physical, since doing so guarantees that our interpretation of our results is sensible. If the frames are physically equivalent then we have exploited the Einstein frame to solve the system, and wasted a few milliseconds transforming back into the Jordan frame. If the frames are **not** equivalent, then we've avoided presenting gibberish. This satisfies both camps.

6.4 Multi-fluid

So far in the thesis we've only looked at single-fluid models, and need to restate a few quantities, now for multi-fluids. In a multi-fluid model, with arbitrary couplings between the fluids, the conservation of the stress-energy tensor take the form, in the Jordan frame, as

$$\nabla^\mu T_{\mu\nu} = \nabla^\mu \sum T^{(A)}_{\mu\nu} = 0, \quad \nabla^\mu T^{(A)}_{\mu\nu} = \mathcal{C}^{(A)}_\nu. \tag{6.1}$$

Transformations into the Einstein frame can be applied to each fluid separately, giving

$$\tilde{\nabla}^\mu \tilde{T}^{(A)}_{\mu\nu} = \tilde{\mathcal{C}}^{(A)}_\nu + \kappa Q \tilde{T}^{(A)} \tilde{\nabla}_\nu \tilde{\phi}. \tag{6.2}$$

The total stress-energy tensor in the Einstein frame, including that for the effective scalar field, is naturally still conserved. We take the matter sector of the Universe to comprise of baryons, cold dark matter (CDM), photons and neutrinos, obeying the Jordan frame conservation laws

$$\nabla^\mu T^{(c)}_{\mu\nu} = 0, \quad \nabla^\mu T^{(\nu)}_{\mu\nu} = 0, \quad \nabla^\mu T^{(b)}_{\mu\nu} = \mathcal{C}^{b\to\gamma}_\nu, \quad \nabla^\mu T^{(\gamma)}_{\mu\nu} = -\mathcal{C}^{b\to\gamma}_\nu. \tag{6.3}$$

[1]Isocurvature in the context of cosmology is the same as entropy perturbations for the fluid we analyze.

[2]This is fine unless we want to do parameter estimation.

In the Einstein frame, these then become

$$\nabla^\mu \tilde{T}^{(c)}_{\mu\nu} = -\kappa Q \rho_c \nabla_\nu \tilde{\phi}, \quad \nabla^\mu \tilde{T}^{(\nu)}_{\mu\nu} = 0, \tag{6.4}$$

$$\nabla^\mu \tilde{T}^{(b)}_{\mu\nu} = \tilde{\mathcal{C}}^{b\to\gamma}_\nu - \kappa Q \rho_b \nabla_\nu \tilde{\phi}, \quad \nabla^\mu \tilde{T}^{(\gamma)}_{\mu\nu} = \tilde{\mathcal{C}}^{\gamma\to b}_\nu, \tag{6.5}$$

where we have used that, for relativistic species, $T = 3p - \rho \equiv 0$ while for dustlike matter $T = -\rho$. Inserting these into the synchronous gauge evolution equations (2.114)-(2.117), we should recover the equations already present in CAMB, adjusted for the awful notation in there. Of note, CAMB's $h' = \frac{\dot{h}}{6}$, and $6h' = 2kz$, so that in our case the z in CAMB is $z = \dfrac{\dot{h}}{2k}$.

6.5 Perturbed FLRW Metric, Jordan and Einstein Frames

6.5.1 Variables in the Jordan and Einstein Frames

To exploit CAMB's existing codes, the system will be solved in the Einstein frame in synchronous gauge. However, it will be necessary to consider the system in the Jordan frame in order to set the initial conditions. Since the initial conditions will be transferred to the Einstein frame, it is then most convenient to express the system in the Jordan frame in conformal Newtonian gauge. In this section, an S denotes synchronous gauge and an N conformal Newtonian; quantities in the Jordan frame are implicitly taken to be in conformal Newtonian gauge.

Remember the full stress-energy tensor of matter in the Jordan frame as

$$T_{\mu\nu} = (\rho + p) u_\mu u_\nu + p g_{\mu\nu} + 2q_{(\mu} u_{\nu)} + \pi_{\mu\nu}. \tag{6.6}$$

The four-velocity and heat flow linearise to

$$u^\mu = \frac{1}{a}(1 - \Phi, v^i), \quad q^\mu = \frac{1}{a}(0, q^i), \tag{6.7}$$

and the anisotropic stress and 3-velocity v^i are linear perturbations. Since we are only considering scalar perturbations these can be written as

$$v^i = \partial^i v \quad \text{and} \quad \pi_{ij} = a^2 (\rho + p) \Big(\partial_i \partial_j - (1/3) \delta_{ij} \partial^l \partial_l \Big) \pi_S. \tag{6.8}$$

Similar definitions apply to the Einstein frame in conformal Newtonian gauge.

The functions of the Ricci scalar in the Jordan frame can be expanded as

$$f \to f + \delta f = f + F \delta R, \quad F \to F + \delta F = F + F_{,R} \delta R, \tag{6.9}$$

with $F_{,R} = dF/dR$. Transforming the stress-energy tensor (6.6) gives

$$\tilde{v}_{Ni} = v_i, \quad \tilde{q}_{Ni} = q_i, \quad \tilde{\pi}_{Ni} = \pi_i, \tag{6.10}$$

while all other relations from equation set (5.23) still hold. The potential linearises to

$$\tilde{V} \to \tilde{V} + \delta\tilde{V}_N = \tilde{V} + \tilde{V}_{,\tilde{\psi}}\delta\tilde{\psi}_N, \tag{6.11}$$

where we have written the scalar field as $\tilde{\psi} = \kappa\tilde{\phi}$ and $\tilde{V}_{,\tilde{\psi}} = dV/d\tilde{\psi}$.

The Einstein frame quantities derived above are in conformal Newtonian gauge. However, in the Einstein frame we will evolve the equations of motion in synchronous gauge, which requires a change of gauge after the conformal transformation. The line element in synchronous gauge (2.90) can be written as

$$d\tilde{s}^2 = \tilde{a}^2(\eta)\left(-d\eta^2 + \left(\left(1 - 2\tilde{\Psi}_S\right)\delta_{ij} + 2\partial_i\partial_j\tilde{E}_S\right)dx^i dx^j\right). \tag{6.12}$$

The transformations from conformal Newtonian gauge to synchronous gauge are given in §2.7.6, while the anisotropic stress is also gauge-invariant.

Our variables differ slightly from those employed by Ma and Bertschinger (with subscript MB), as well as Bean and Pogosian [21, 53], in the manner

$$k^2 v = -\theta_{\mathrm{MB}}, \tag{6.13}$$

$$2k^2\pi_S = 3\sigma_{\mathrm{MB}}, \tag{6.14}$$

$$\Psi = \eta_{\mathrm{MB}}, \tag{6.15}$$

$$2k^2 E = -(h_{\mathrm{MB}} + 6\eta_{\mathrm{MB}}). \tag{6.16}$$

Our π_S is related to Π in [18] by $\Pi = (\rho + p)\pi_S$. Photons and neutrinos are not perfect fluids, although while photons are tightly-coupled to baryons they can be described as such. Instead, these fluids are described by distributions functions; with the momentum dependence integrated out these are "brightness functions". We consider the transformation of the brightness function in §6.5.3.

6.5.2 Equations of Motion

An index i runs across all matter, r runs across radiative matter and m across dustlike matter. The effective scalar field in the Einstein frame will always be written explicitly and never included in such a sum. Henceforth, unless otherwise noted, quantities in the Einstein frame are in synchronous gauge, while those in the Jordan frame are in conformal Newtonian gauge. In the Jordan frame the background Einstein field equations are

$$3\left(\frac{\dot{a}}{a}\right)^2 + \frac{a^2}{2}\frac{f}{F} - 3\frac{\ddot{a}}{a} + 3\frac{\dot{a}}{a}\frac{\dot{F}}{F} = \frac{a^2\kappa^2}{F}\sum_i \rho_i, \tag{6.17}$$

$$\frac{\ddot{a}}{a} + \left(\frac{\dot{a}}{a}\right)^2 - \frac{\ddot{F}}{F} - \frac{\dot{a}}{a}\frac{\dot{F}}{F} - \frac{a^2}{2}\frac{f}{F} = \frac{a^2\kappa^2}{F}\sum_i p_i. \tag{6.18}$$

Matter follows as always

$$\dot{\rho} + 3\mathcal{H}(1 + w)\rho = 0. \tag{6.19}$$

The Friedmann equations in the Einstein frame are simply

$$3\left(\frac{\dot{\tilde{a}}}{\tilde{a}}\right)^2 = \tilde{a}^2\kappa^2\left(\sum_i \tilde{\rho}_i + \tilde{\rho}_\phi\right), \quad 2\frac{\ddot{\tilde{a}}}{\tilde{a}} - \left(\frac{\dot{\tilde{a}}}{\tilde{a}}\right)^2 = -\tilde{a}^2\kappa^2\left(\sum_i \tilde{p}_i + \tilde{p}_\phi\right), \tag{6.20}$$

where

$$\kappa^2\tilde{\rho}_\phi = \frac{1}{2\tilde{a}^2}\dot{\tilde{\psi}}^2 + \kappa^2\tilde{V}(\tilde{\psi}), \quad \kappa^2\tilde{p}_\phi = \frac{1}{2\tilde{a}^2}\dot{\tilde{\psi}}^2 - \kappa^2\tilde{V}(\tilde{\psi}). \tag{6.21}$$

The Klein-Gordon equation for the scalar field becomes

$$\ddot{\tilde{\psi}} + 2\tilde{\mathcal{H}}\dot{\tilde{\psi}} + \tilde{a}^2\kappa^2\tilde{V}_{\tilde{\phi}} = -\tilde{a}^2\kappa^2 Q\sum_i\left(\tilde{\rho}_i - 3\tilde{p}_i\right) = -\tilde{a}^2\kappa^2 Q\sum_m \tilde{\rho}_m, \tag{6.22}$$

and matter continuity is

$$\dot{\tilde{\rho}}_m + 3\tilde{\mathcal{H}}\tilde{\rho}_m = Q\tilde{\rho}_m\dot{\tilde{\psi}}, \quad \dot{\tilde{\rho}}_r + 4\tilde{\mathcal{H}}\tilde{\rho}_r = 0. \tag{6.23}$$

Remember that the functions of the Ricci scalar in the Jordan frame can be expanded as

$$f \to f + F\delta R, \quad F(R) = F + F_{,R}\delta R. \tag{6.24}$$

The perturbed Einstein equations in the Jordan frame can then be written in Fourier space [53] as

$$\dot{\delta}_b - k^2 v_b - 3\dot{\Psi} = \delta\mathcal{C}_0^{b\to\gamma}, \qquad \dot{\delta}_\gamma - \frac{4}{3}k^2 v_\gamma - 4\dot{\Psi} = -\delta\mathcal{C}_0^{b\to\gamma}, \tag{6.25}$$

$$\dot{v}_b + \mathcal{H}v + \Phi = \delta\mathcal{C}_i^{b\to\gamma}, \qquad \dot{v}_\gamma + \frac{1}{4}\delta_\gamma + \Phi - \frac{2}{3}k^2\pi_{S\gamma} = -\delta\mathcal{C}_i^{b\to\gamma} \tag{6.26}$$

$$\begin{aligned} &6\mathcal{H}\left(\dot{\Psi} + \mathcal{H}\Phi\right) + 2k^2\Psi + 3\frac{F_{,R}}{F}\dot{\mathcal{H}}\delta R - k^2\frac{F_{,R}}{F}\delta R \\ &- 3\frac{\mathcal{H}}{F}\frac{\partial}{\partial\eta}\left(F_{,R}\delta R\right) + \dot{F}\left(6\mathcal{H}\Phi + 3\dot{\Phi}\right) = -a^2\kappa^2\sum_i \rho_i\delta_i, \end{aligned} \tag{6.27}$$

$$F\left(\Phi - \Psi\right) + F_{,R}\delta R = -\frac{4}{3}a^2\kappa^2\left(\rho_\gamma\pi_{S\gamma} + \rho_\nu\pi_{S\nu}\right), \tag{6.28}$$

where matter continuity is unchanged from general relativity. To find the CDM and neutrino equations, take the baryon and photon equations with $\delta\mathcal{C}_\mu = 0$. The perturbed Ricci scalar is the perturbation part of equation (2.100),

$$\delta R = -\frac{2}{a^2}\left(6\frac{\ddot{a}}{a}\Phi + 3\mathcal{H}\dot{\Phi} - k^2\Phi + 9\mathcal{H}\dot{\Psi} + 3\ddot{\Psi} + 2k^2\Psi\right). \tag{6.29}$$

The perturbation equations in the Einstein frame are those of general relativity in the presence of a quintessence field coupled to dustlike matter. In the Einstein frame, in synchronous gauge, the perturbed Einstein equations then become [53],

$$3\tilde{\mathcal{H}}\dot{\tilde{\Psi}} + k^2\left(\tilde{\Psi} + \tilde{\mathcal{H}}\dot{\tilde{E}}\right) = -\frac{\tilde{a}^2\kappa^2}{2}\sum_i \tilde{\rho}_i\tilde{\delta}_i - \frac{1}{2}\left(\dot{\tilde{\psi}}\delta\dot{\tilde{\psi}} + \kappa^2 V_\psi \delta\psi\right), \tag{6.30}$$

$$\dot{\tilde{\Psi}} = -\frac{\tilde{a}^2\kappa^2}{2}\tilde{\rho}\tilde{v} + \frac{1}{2}\dot{\tilde{\psi}}\delta\psi, \tag{6.31}$$

$$\ddot{\tilde{\Psi}} + 2\tilde{\mathcal{H}}\dot{\tilde{\Psi}} = \frac{\tilde{a}^2\kappa^2}{2}\left(\tilde{c}_s{}^2\tilde{\rho}\tilde{\delta} - \frac{8}{3}k^2\tilde{\rho}\tilde{\pi}\right) + \frac{1}{2}\left(\dot{\tilde{\psi}}\delta\dot{\tilde{\psi}} - \kappa^2 V_\psi \delta\tilde{\psi}\right), \tag{6.32}$$

$$\ddot{\tilde{E}} + 2\tilde{\mathcal{H}}\dot{\tilde{E}} + \tilde{\Psi} = (1+w)\tilde{a}^2\kappa^2\tilde{\rho}\tilde{\pi}, \tag{6.33}$$

while matter continuity for a fluid with arbitrary scatterings is

$$\dot{\tilde{\delta}} + 3\tilde{\mathcal{H}}\left(\tilde{c}_s{}^2 - w\right)\tilde{\delta} - (1+w)\left(k^2(\tilde{v} + \dot{\tilde{E}}) + 3\dot{\tilde{\Psi}}\right) = \tilde{\mathcal{C}}_0 - Q(1-3w)\left(\dot{\tilde{\psi}}\tilde{\delta} + \delta\dot{\tilde{\psi}}\right), \tag{6.34}$$

$$\dot{\tilde{v}} + \left(1 - 3\tilde{c}_s{}^2\right)\tilde{\mathcal{H}}\tilde{v} + \left(\frac{\tilde{\delta p}}{\tilde{\rho}+\tilde{p}} - \frac{2}{3}k^2\pi_S\right) = \tilde{\mathcal{C}}_i. \tag{6.35}$$

Inserting the various fluids, these translate to

$$\dot{\tilde{\delta}}_b - k^2\left(\tilde{v}_b + \dot{\tilde{E}}\right) - 3\dot{\tilde{\Psi}} = \delta\tilde{\mathcal{C}}_0^{b\to\gamma} - Q\left(\dot{\tilde{\psi}}\delta_b + \delta\dot{\tilde{\psi}}\right), \tag{6.36}$$

$$\dot{\tilde{\delta}}_\gamma - \frac{4}{3}k^2\left(\tilde{v}_\gamma + \dot{\tilde{E}}\right) - 4\dot{\tilde{\Psi}} = -\delta\tilde{\mathcal{C}}_0^{b\to\gamma}, \tag{6.37}$$

$$\dot{\tilde{v}}_b + \tilde{\mathcal{H}}v_b = \delta\tilde{\mathcal{C}}_i^{b\to\gamma}, \quad \dot{\tilde{v}}_\gamma + \frac{1}{4}\tilde{\delta}_\gamma - \frac{2}{3}k^2\pi_\gamma = -\delta\tilde{\mathcal{C}}_i^{b\to\gamma}, \tag{6.38}$$

where neutrino and CDM equations of motion again are found by taking $\delta\tilde{\mathcal{C}}_\mu = 0$ in the photon and baryon expressions. The scalar field itself obeys the perturbed Klein-Gordon equation

$$\delta\ddot{\tilde{\psi}} + 2\tilde{\mathcal{H}}\delta\dot{\tilde{\psi}} + \left(k^2 + \tilde{a}^2\kappa^2 V_{,\psi\psi}\right)\delta\tilde{\psi} = \left(3\dot{\tilde{\Psi}} + k^2\dot{\tilde{E}}\right)\dot{\psi} - \tilde{a}^2\kappa^2 Q\left(\tilde{\rho}_b\tilde{\delta}_b + \tilde{\rho}_c\tilde{\delta}_c\right). \tag{6.39}$$

We therefore have to add the potential and couplings to the scalar field to the code.

6.5.3 Observables: The CMB Angular Power Spectrum

The angular power spectrum of the temperature auto-correlation is given in the Jordan frame by,

$$C_l = \frac{1}{8\pi}\int \mathcal{P}(k)\left|\Delta_{Tl}(k,\eta_0)\right|^2\frac{dk}{k}, \tag{6.40}$$

where the photon transfer functions $\Delta_{Tl}(k,\eta_0)$ are the moments of the photon brightness function at the present epoch separated across the Legendre polynomials and $\mathcal{P}(k)$ the primordial power spectrum. It is these transfer functions that a Boltzmann code is designed to calculate. We therefore need to know how the brightness function transforms between the Einstein and the Jordan frames. Fortunately, this is quick to find. Note first that [102]

$$\Delta_{T0} = \delta_\gamma, \quad \Delta_{T1} = -\frac{4}{3}kv_\gamma, \quad \Delta_{T2} = \frac{3}{k^2}\pi_S. \tag{6.41}$$

Then we immediately have

$$\tilde{\Delta}_{T0} = \Delta_{T0} - 2\frac{\delta F}{F}, \quad \tilde{\Delta}_{T1} = \Delta_{T1}, \quad \tilde{\Delta}_{T2} = \Delta_{T3}. \tag{6.42}$$

When separated across the Legendre polynomials the Boltzmann equation becomes an infinite hierarchy of equations, with each moment coupling to the ones above and below. Neglecting for simplicity the couplings, for $l \geq 2$ in conformal Newtonian gauge the Boltzmann hierarchy is [21]

$$\dot{\Delta}_{Tl} = \frac{k}{2l+1}\left(l\Delta_{Tl-1} - (l+1)\Delta_{Tl+1}\right), \tag{6.43}$$

and takes the same form in both frames. We immediately conclude that

$$\tilde{\Delta}_{Tl} = \Delta_{Tl}, \quad l \geq 2, \tag{6.44}$$

with the proof by induction. The same arguments apply for the case with couplings, and for the polarization hierarchies. To find the CMB angular power spectrum, then, we can simply evaluate it in the Einstein frame at the end of a calculation; so long as we calculate it at the correct Einstein frame scale factor, the observables do not change. Similar arguments apply to the higher order moments of the CMB such as the angular bispectrum. Note that the transfer functions are solved by an integral of the form $\Delta_{Tl} \propto \int S_T(k,\eta)j_l(k(\eta-\eta_0))d\eta$, whose time-dependence might lead one to assume that we cannot simply solve in the Einstein frame in the method we propose. However, this time dependence is entirely carried on the scale factor, whose behaviour in the two frames is well understood, and on the conformal time, which is invariant between the frames.

6.6 Initial Conditions

As we will consider the Jordan frame to be the "physical" one, we will first find the initial conditions here.

6.6.1 Background Initial Conditions in the Jordan Frame

We set the initial conditions at $a_0 = 1$ in the Jordan frame, and wish to set all quantities by the background terms $\{\Omega_{b0}, \Omega_{c0}, T_{\mathrm{CMB}}, \mathcal{H}_0, q_0\}$. The subscript 0 denote present day values. We start out with reminding you of the definition of the density parameter in the Jordan frame,

$$\Omega_{i0} = \frac{\kappa^2\rho_{i0}}{3F_0\mathcal{H}_0^2}, \tag{6.45}$$

where F_0 is the initial condition of F, given as $F(R_0)$. This gives us

$$\kappa^2 \rho_{i0} = 3F_0 \mathcal{H}_0^2 \Omega_{i0} \tag{6.46}$$

for each type of fluid. Since we assume a flat background the effective energy density of the modified gravity terms is then,

$$\Omega_{F0} = 1 - \Omega_{b0} - \Omega_{c0}, \tag{6.47}$$

the photon energy density is $\rho_{\gamma 0} = (\pi^2/30) g_\star^\gamma T_{\mathrm{CMB}}^4$ and the neutrino energy density is $\rho_{\nu 0} = (7/8) N_\nu (4/11)^{4/3} T_{\mathrm{CMB}}^4$, which give us [103]

$$\Omega_{\gamma 0} \approx \left(2.48 \times 10^{-5}\right) h^{-2} F_0^{-1}, \quad \Omega_{\nu 0} \approx 1.68 \Omega_{\gamma 0}. \tag{6.48}$$

Contrary to standard practice we specify the current behaviour of the modifications with the deceleration parameter q_0 rather than an effective equation of state. From the definition of the deceleration parameter we can find initial conditions for the term $\frac{\ddot{a}}{a}$,

$$\begin{aligned} q &= -\frac{\dot{\mathcal{H}}}{\mathcal{H}^2} = 1 - \frac{\ddot{a}}{a\mathcal{H}^2} \\ \Rightarrow & \boxed{\left.\frac{\ddot{a}}{a}\right|_0 = (1 - q_0)\mathcal{H}_0^2}. \end{aligned} \tag{6.49}$$

With this initial condition, we can set up the initial condition of the Ricci scalar

$$\begin{aligned} R &= \frac{6}{a^2} \frac{\ddot{a}}{a} \\ \Rightarrow & \boxed{R_0 = \frac{6}{a_0^2}(1 - q_0)\mathcal{H}_0^2}. \end{aligned} \tag{6.50}$$

Now we are only left with the initial conditions for $\frac{\dot{F}}{F}$, which we can get by using all of the above initial conditions alongside equation (3.11),

$$\begin{aligned} 3\mathcal{H}_0 \left.\frac{\dot{F}}{F}\right|_0 &= \frac{a_0^2 \kappa^2 \rho_{m0}}{F_0} + 3\left.\frac{\ddot{a}}{a}\right|_0 - \frac{a_0^2}{2}\frac{f_0}{F_0} - 3\mathcal{H}_0^2 \\ \Rightarrow & \boxed{\left.\frac{\dot{F}}{F}\right|_0 = \mathcal{H}_0 \left(\Omega_{m0} - q_0\right) - \frac{1}{6\mathcal{H}_0}\frac{f_0}{F_0}}. \end{aligned} \tag{6.51}$$

From these initial conditions we can extract the parameters we require, $\tilde{a}_0$, $\tilde{\mathcal{H}}_0$, $\tilde{\rho}_{i0}$, $\tilde{\psi}_0$ and $\dot{\tilde{\psi}}_0$ in the Einstein frame.

6.6.2 Background Initial Conditions in the Einstein Frame

We find the initial conditions in the Einstein frame by immediately performing the transformation from equation set (5.23),

$$\tilde{a}_0 = \sqrt{F_0}a_0 \Rightarrow \boxed{\tilde{a}_0 = \sqrt{F_0}}, \tag{6.52}$$

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0 + \frac{1}{2}\frac{\dot{F}}{F}\bigg|_0 \Rightarrow \boxed{\tilde{\mathcal{H}}_0 = \mathcal{H}_0 + \frac{1}{2}\mathcal{H}_0\left(\Omega_{m0} - q_0\right) - \frac{1}{12\mathcal{H}_0}\frac{f_0}{F_0}}, \tag{6.53}$$

$$\kappa^2\tilde{\rho}_{m0} = \frac{\kappa^2\rho_{m0}}{F_0^2} \Rightarrow \boxed{\kappa^2\tilde{\rho}_{m0} = \frac{3\mathcal{H}_0^2\Omega_{m0}}{F_0}}. \tag{6.54}$$

Note that we are ending our integration with $\tilde{a} > 0$ in contrast to the usual $\tilde{a} = 1$, a point we had to be aware of in order to make sure our modifications are robust enough to handle this change. Finally we need the initial condition for the scalar field and the potential. We again redefine $\tilde{\psi} = \kappa\tilde{\phi}$ and the initial conditions follow seamlessly,

$$\tilde{\psi}_0 = -\frac{1}{2Q}\ln F_0, \tag{6.55}$$

$$\dot{\tilde{\psi}}_0 = \frac{1}{2Q}\left(\frac{1}{6\mathcal{H}_0}\frac{f_0}{F_0} - \mathcal{H}_0\left(\Omega_{m0} - q_0\right)\right), \tag{6.56}$$

$$\kappa^2\tilde{V}_0 = \frac{6H_0^2(1-q_0)F_0 - f_0}{2F_0^2}. \tag{6.57}$$

The energy density and equation of state of the scalar field are then given by,

$$\kappa^2\tilde{\rho}_{\phi 0} = \frac{1}{2\tilde{a}_0^2}\dot{\tilde{\psi}}_0 + \kappa^2\tilde{V}_0 \quad \text{and} \quad \tilde{w}_{\phi 0} = \frac{\dot{\tilde{\psi}}_0^2 - 2\tilde{a}_0^2\kappa^2\tilde{V}_0}{\dot{\tilde{\psi}}_0^2 + 2\tilde{a}_0^2\kappa^2\tilde{V}_0}. \tag{6.58}$$

Equations (6.55) and (6.58) give us the constraints at the current epoch. However the evolution equation for the scalar field will generically possess a growing and a decaying mode [3]. If we simply integrate the conditions above backwards, then, we will typically encounter the decaying mode, which will drive us far from the matter- and radiation-dominated backgrounds we want for a valid cosmology. In the language of dynamical systems theory [104, 105, 106], we want to ensure that we follow a trajectory from near a fixed point associated with radiation, past a fixed point associated with matter, and towards a fixed point associated with vacuum domination.

We therefore need to set initial conditions at some early scale factor $\tilde{a} \sim 10^{-8}$, and in principle this requires fixing $\{\Omega_b, \Omega_c, \Omega_\gamma, \Omega_\nu, \tilde{\psi}, \dot{\tilde{\psi}}\}$ at the early time, and hunting through this parameter space for a combination which results in a viable cosmology. In standard quintessence, the matter and radiation densities have a trivial dependence on scale factor, which along with setting $\dot{\tilde{\psi}}_i = 0$,[3] reduces the number of parameters in

[3]We know that $\tilde{\psi}$ is going to be small, and can therefore deduce that its derivative will be vanishingly small as well. This is also what is done in the quintessence module in vanilla CAMB [87].

the space to one, $\tilde{\psi}$, which is quickly explored. The situation in coupled quintessence scenarios (including extended gravities in the Einstein frame) is more complicated, since the matter densities do not evolve trivially with scale factor. However, following [34] we can solve equation (6.19) to formally give

$$\tilde{\rho}_m(\tilde{a}) = \tilde{\rho}_{m0}\left(\frac{\tilde{a}_0}{\tilde{a}}\right)^{3(1+w)} \exp\left(Q(\tilde{\psi}(\tilde{a}) - \tilde{\psi}_0)\right). \tag{6.59}$$

This allows us to again reduce the parameter space at $\tilde{a} \approx 10^{-8}$ to the single variable $\tilde{\psi}$. At each stage, when $\tilde{\psi}$ has been propagated to the current epoch, $\tilde{\rho}_{\phi 0}$ and $\tilde{w}_{\phi 0}$ can be calculated and compared with the desired parameters, making them essentially boundary conditions rather than initial conditions.

6.6.3 Initial Conditions for Linear Perturbations

The initial conditions for the cosmological perturbations are set on superhorizon scales in the very early universe. We will not focus much attention on the initial conditions, as they in general are extremely model-dependent, and one of the greatest efforts in employing a Boltzmann code in the Einstein frame will be in finding suitable initial conditions for the perturbations. Since we aim towards using $f(R)$ models as a simple test case, we will not concern ourselves in this section with finding specific initial conditions for specific models and instead consider the generic effects that one should expect to occur.

Without requiring us to yet choose a model let us assume that the standard GR initial conditions in [21] hold. These are:

$$\Phi = \frac{20C}{15 + 4R_\nu}, \quad \Psi = \left(1 + \frac{2R_\nu}{5}\right)\Phi, \quad \delta_\gamma = \delta_\nu = \frac{4}{3}\delta_b = \frac{4}{3}\delta_c = -2\Phi, \tag{6.60}$$

$$v_\gamma = v_\nu = v_b = v_c = -\frac{1}{2}\Phi\eta, \quad \pi_\nu = \frac{1}{12}\Phi\eta^2, \tag{6.61}$$

where $R_\nu = \rho_\nu/\rho_r$ is a constant, $R_\nu \approx 0.25$. Using that[4] $\delta R \approx -2\Phi R$ then gives the Einstein frame initial conditions:

$$\begin{gathered}\tilde{\Phi} = \Phi\left(1 - R\frac{F_{,R}}{F}\right), \quad \tilde{\Psi} = \Phi\left(1 + \frac{2}{5}R_\nu + R\frac{F_{,R}}{F}\right), \\ \tilde{\delta}_\gamma = \tilde{\delta}_\nu = -2\Phi\left(1 - 2R\frac{F_{,R}}{F}\right), \quad \tilde{\delta}_b = \tilde{\delta}_c = -2\Phi\left(\frac{3}{4} - 2R\frac{F_{,R}}{F}\right), \\ \tilde{v}_i = v_i, \quad \tilde{\pi}_\nu = \pi_\nu, \quad \delta\psi = R\frac{F_{,R}}{F}\Phi.\end{gathered} \tag{6.62}$$

We can then immediately see that the system in the Einstein frame has in principle a large amount of isocurvature, which arises from the effective isocurvature in the Jordan

[4] This approximation comes from taking equation (6.29) and treating Φ and Ψ as constants and dropping all terms proportional to k.

frame between the matter perturbations and the geometry. As the CMB is frame-independent, we therefore would expect the CMB angular power spectrum generated in arbitrary models of extended gravity to resemble qualitatively CMB angular power spectra from models with significant isocurvature, such as coupled multi-field inflation [107, 108]. However, the initial conditions here are perhaps more surprising than those in such models; in those cases one retains relatively straightforward relationships between the gravitational potentials and the matter perturbations. Here, not only are the relationships between the potentials violated, but so also are all the relationships with the density contrasts.

It is also worth noting that the errors induced by the transformations when not working within the restricted set of gauges or properly dealing with the extra degrees of freedom, will be at the order of the deviation from standard GR. In this specific model the deviations are low, and would not cause much of a problem, but principally we do not know how big these deviations are for other extended gravity theories. However, however small the errors might be at the initial conditions, we do not know how much they will compound as the equations are evolved, and care should always be taken.

6.7 Constraints on $f(R)$ Gravity Theories

By choosing to work with the initial conditions that work for GR we restrict our choices of what $f(R)$ theories will be allowed for us to put into our modified code at this point. In this section we will briefly look at certain criteria that $f(R)$ gravity theories need to fulfill.

6.7.1 Demanding a Radiation Dominated Past

We take "radiation domination" to imply $\rho_r \gg \rho_m$ – in the case of GR, this additionally implies that $a \propto \eta$. At early times there will be a period that is almost indistinguishable from standard GR. In these cases, at very early times we can write $f(R) \approx R + g(R)$ where $g(R) \ll R$, and the initial conditions to be as in GR [21, 19] (potentially with small corrections).

Note that in principle it is not necessary that we possess a radiation dominated era; we can insert any modified gravity we wish into the code and examine its evolution. However, any model which does not possess a radiation-dominated era at early times – whether or not it then passes into a matter dominated era – will require much additional study to set the initial conditions for the perturbations. For convenience, we restrict ourselves to models which indeed pass extremely close to a radiation dominated era, in which case the perturbations will behave as their GR counterparts would.

Assuming radiation domination and that $a \propto \eta^{1+\epsilon}$ (with ϵ not necessarily small or positive), the Friedmann equations give

$$\ddot{G} - \frac{2(1+\epsilon)}{\eta}\dot{G} - \frac{2(2+\epsilon)(1+\epsilon)}{\eta^2}(1+G) = -\frac{4}{3\eta^{2(1+\epsilon)}}\frac{\kappa^2 \rho_{rI}}{a_I^2} = \frac{\mathcal{C}}{\eta^{2(1+\epsilon)}}, \qquad (6.63)$$

where $G(R) = g_{,R}(R)$. Surprisingly, this has the general solution of

$$G(\eta) = \frac{4 - \mathcal{C}\eta^{-2\epsilon} - 6\epsilon^2}{6\epsilon^2 - 4} + A\eta^{(3+2\epsilon-\sqrt{25+36\epsilon+12\epsilon^2})/2} + B\eta^{(3+2\epsilon+\sqrt{25+36\epsilon+12\epsilon^2})/2}. \quad (6.64)$$

This is a general condition for the behaviour of $f(R)$ if one wishes a power-law radiation era. Restricting to $\epsilon \ll 1$ gives us a radiation domination with a similar scaling to standard GR, for which the modified gravity must satisfy

$$F(\eta) \approx \frac{1}{4}\mathcal{C}\left(1 - 2\epsilon \ln \eta\right) + \frac{A}{\eta}\left(1 - \frac{4}{5}\epsilon \ln \eta\right) + B\eta^4\left(1 + \frac{14}{5}\epsilon \ln \eta\right). \quad (6.65)$$

We set $\epsilon = 0$ in equation (6.64) and get a condition to satisfy pure radiation domination

$$G(\eta) = \frac{\mathcal{C} - 4}{4} + A\eta^{-1} + B\eta^4. \quad (6.66)$$

We leave normalizing this constraint for future work.

6.7.2 Constraints from the Initial Conditions

We can get more constraints from the initial conditions worked out above, by inserting them into the various Einstein equations. First off, we insert the initial conditions into

$$F(\Phi - \Psi) + F_{,R}\delta R = -\frac{4a^2\kappa^2}{3}\rho_\nu \pi_\nu,$$

and get

$$R\frac{F_{,R}}{F} = \frac{\Omega_{\nu 0} F_0 \mathcal{H}_0^2 \eta^2}{6F} - \frac{R_\nu}{5}. \quad (6.67)$$

Likewise we can find a constraint by inputting the initial conditions into the other field equation; however it will result in higher order derivatives of a, so we will not consider it at the time being. Should and $f(R)$ model satisfy these constraints we can use the Ma and Bertschinger conditions.

6.8 Numerical Methods

We have for the most part only been using the numerical methods found in the original CAMB, with a few exceptions. For one part of the code we've turned to Numerical Recipes, and modified their routine *Miser*. Miser is a Monte Carlo algorithm by Press and Farrar [109] that is based on recursive stratified sampling [110]. See the mentioned citations for an in depth overview of Miser and Monte Carlo in general. For our purpose it is enough to state that Monte Carlo is a well tested and very flexible integration method that utilizes random numbers. It analyzes integrals on a grid, by choosing a random point at which to evaluate the integrand.

6.9 Structure of Our Code

As well as the modifications mentioned above, we have made several structural changes and additions to CAMB.

- Added an $f(R)$ module that give user specified $f(R)$, $F(R)$, $F_{,R}(R)$, $V(\tilde{\phi})$, $V_{,\tilde{\phi}}(\tilde{\phi})$, $V_{,\tilde{\phi}\tilde{\phi}}(\tilde{\phi})$ and initial conditions.
- A background module evaluating the Einstein frame background assuming the inputs are given in the Jordan frame.
- We have modified the code throughout to propagate this background, note that these modifications are everywhere.
- Added perturbation support for coupled scalar fields.
- And finally output C_l, Δ_{Tl}, Δ_{Bl} and Δ_{El} to file, output of the matter density contrast δ_m is to be added later.

6.10 Summarizing

In this chapter we have shown the concept of how we wish the modified code to function:

1. Set up initial conditions in Jordan frame in conformal Newtonian gauge.
2. Transform to Einstein frame.
3. Refix to synchronous gauge.
4. Evolve the evolution equations from a distant past to what is equivalent to today in the Jordan frame.
5. Finally transforming back to conformal Newtonian gauge and the Jordan frame for constructing the observables.

We've also supplied all the evolution equations that the code need, and touched upon the various constraints imposed on our $f(R)$ theory by choosing to work with Ma and Bertschinger's initial conditions. However in its final form we wish the code to be able to handle **any** extended gravity theory that has an Einstein frame representation, not only $f(R)$ theories. This will however entail theoretical effort before the code can be employed.

Once the code is finished we wish to employ all the various $f(R)$ theories discussed in §3.4; however for the time being we'll be working in the simple, and arguably best, $f(R)$ theory, the Starobinsky model. The reason for this choice is that it is simple, so that we in fact can continue with analyzing the non-Gaussianity parameter $f_{\rm NL}$ without the code being in a complete tested form. We can do this as when using this model and the statistics derived in Chapter 4, our code simplifies down to vanilla CAMB and we can go ahead with the analysis.

At the time of writing the code is nearing completion, and work will continue immediately after this thesis is finished and defended. The code should be finished in the near future, and a paper should follow soon after.

Chapter 7

Results in $f(R)$ inflation

In this chapter we will provide the results we can produce from the previous chapters. First and foremost, we return to Chapter 4, to analyze the behaviour of the non-Gaussianity parameter f_{NL} for a specific model.

7.1 The Return of $f(R) = R + \alpha R^2$

We return to Starobinsky's inflation model with $\alpha = (6M^2)^{-1}$, where M is given by the Planck mass m_{Pl}. This model has been extensively researched, most notably for our purposes by Hwang and Noh [56] and Tsujikawa and De Felice [2]. Let us first note that this model is almost indistinguishable from the ΛCDM model with an $m_{Pl}^2\phi^2$ potential. We continue by noting that our slow-roll parameters from Chapter 4 differ from theirs in the manner

$$\epsilon_1 = -\epsilon_1^{HN} = \epsilon_1^{TF}, \quad \epsilon_2 = 2\epsilon_3^{HN} = 2\epsilon_3^{TF}, \quad \epsilon_3 = \epsilon_4^{HN} = \epsilon_4^{TF}. \tag{7.1}$$

As shown in Tsujikawa and De Felice's general overview of $f(R)$ models, and originally derived by Hwang and Noh, these slow-roll parameters give the spectral index of the primordial power spectrum, and the tensor/scalar ratio (as derived by Hwang and Noh),

$$n_S - 1 \approx -4\epsilon_1, \quad r \approx 48\epsilon_1^2. \tag{7.2}$$

Here, $\epsilon_3 \approx -\epsilon_1$ and $\epsilon_2 \approx -2\epsilon_1$ has been used, justified in [56]. It is also shown that these slow roll parameters can be related to the number of e-foldings (2.70) as

$$\epsilon_1 \approx \frac{1}{2N}, \quad \epsilon_2 \approx -\frac{1}{N}, \quad \epsilon_3 \approx -\frac{1}{2N}, \tag{7.3}$$

implying

$$n_S \approx 1 - \frac{2}{N} = 1 - 3.6 \times 10^{-2}\left(\frac{55}{N}\right), \quad r \approx \frac{12}{N^2}, \tag{7.4}$$

where the odd approximation of $2 \approx 3.6 \times 10^{-2} \cdot 55$ has been used since we can assume $N \approx 55$, which would give us

$$n_S \approx 0.964, \quad r \approx 4 \times 10^{-3}.$$

This spectral index has a value square in the middle of the region allowed by WMAP-7 [24], while the tensor/scalar ratio would indicate a very low background of gravitational waves. It can further be shown that for this model [56],

$$\alpha \approx 1.5 \times 10^{12} m_{Pl}^2. \tag{7.5}$$

With this value of α, inflation has long since ended and a suitable period of reheating has occurred[1], so that we don't even need our extensive modifications to CAMB. Instead, we merely need to insert the amplitude of the primordial perturbations and the spectral index to recover a CMB angular power spectrum extremely close to the standard ΛCDM model. More interestingly, we will recover a B-mode angular power spectrum significantly lower than is frequently assumed; $r \lesssim 0.1$ is still allowed by the data [24], and it is typical to push r as high as is allowed.

At this point we will need to start looking at the various k-configurations introduced in §4.5.2; however in order to simplify the choice of configurations we can use the parametrization

$$\begin{aligned} k_2 &= \beta k_1, \\ k_3^2 &= k_1^2 \left(1 + \beta^2 + 2\beta\cos\phi\right). \end{aligned} \tag{7.6}$$

In this parametrization[2];

- Equilateral configuration corresponds to $\beta = 1$ and $\phi = \dfrac{2\pi}{3}$.
- Squeezed configuration corresponds to $\beta = 1$ and $\phi = \pi$.
- Colinear configuration corresponds to $\beta = 1$ and $\phi = 0$.

With this parametrization we have reduced the 3-dimensional $f_{\rm NL}(k_1, k_2, k_3)$ to a 2-dimensional surface $f_{\rm NL}(\beta, \phi)$. Specializing these to the colinear, equilateral and squeezed configurations gives,

$$\begin{aligned} f_{\rm NL}^{\rm Col} &= \frac{23}{48}D_1 - \frac{10}{3}D_2 + \frac{1}{24}D_3 + \frac{1}{12}D_4, \\ f_{\rm NL}^{\rm Eq} &= \frac{20}{27}D_1 - \frac{10}{3}D_2 + \frac{20}{27}D_3 - \frac{20}{27}D_4, \\ f_{\rm NL}^{\rm Sq} &= \frac{5}{12}D_1 - \frac{10}{3}D_2; \end{aligned} \tag{7.7}$$

[1] It was shown in Hwang and Noh [56], that this arises automatically. As well as in [111] for a modification of this model.

[2] It is also important to note that $\beta \to \infty$ corresponds to a rotation of the squeezed configuration, implying $k_1 \to 0$.

for an arbitrary configuration $f_{\rm NL}^{\rm Arb}$, see Appendix B. We find an approximation to the non-linearity parameter by using the fact that the slow-roll parameters are small, and that $\epsilon_2 = 2\epsilon_3$, and drop everything down to leading order. This leaves us with

$$f_{\rm NL,approx} = -\frac{10}{3} D_2, \tag{7.8}$$

as an approximation to the non-linearity parameter. Whether or not this is a good approximation we will see shortly. In order to see if equilateral is dominating or not, we use that $\epsilon_3 = \epsilon_2/2$, $\epsilon_2 = -1/N$ and equation set (7.7) so that

$$\frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Col}} = \frac{10\left(10N^2 - 22N + 5 + 16N^3\right)}{(2N-1)^2(40N+43)}, \quad \frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Sq}} = \frac{1}{4}\frac{10N^2 - 22N + 5 + 16N^3}{(N+1)(2N-1)^2}, \tag{7.9}$$

and a corresponding form for the ratio of the equilateral line to an arbitrary line. In the limit $N \to \infty$, then, we see

$$\frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Col}} = \frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Sq}} = 1. \tag{7.10}$$

Even for $N = 1$, which would be a very puny inflationary era, we see that

$$\frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Col}} = \frac{90}{83}, \quad \frac{f_{\rm NL}^{\rm Eq}}{f_{\rm NL}^{\rm Sq}} = \frac{9}{8}, \tag{7.11}$$

and the f_{NL} parameters for different configurations are of the same order-of-magnitude. This suggests that the f_{NL} parameter is approximately a constant. Inserting this into equation set (7.7) we get

$$f_{\rm NL}^{\rm Col} \approx 15.73 \times 10^{-3}, \tag{7.12}$$

$$f_{\rm NL}^{\rm Eq} \approx 15.89 \times 10^{-3}, \tag{7.13}$$

$$f_{\rm NL}^{\rm Sq} \approx 15.71 \times 10^{-3}, \tag{7.14}$$

and from equation (7.8),

$$f_{\rm NL,approx} \approx 15.61 \times 10^{-3}. \tag{7.15}$$

We note that all of these values are within the current bounds for the non-linearity parameter set up by WMAP 7, e.g. $f_{\rm NL}^{\rm Eq} \in (-214, 266)$ and $f_{\rm NL}^{\rm Sq} \in (-10, 74)$ [24]; we expect much tighter constraints from Planck once the data is released to the public.

7.1.1 Results for the Power Spectrum

As we found above, this model has a spectral index $n_S \approx 0.964$ and we can therefore find the power spectrum of this mode simply by using CAMB to calculate the C_l for this n_S. In Figure 7.1 we show the power spectrum for this model, as well as the Harrison-Zel'dovich angular power spectrum.

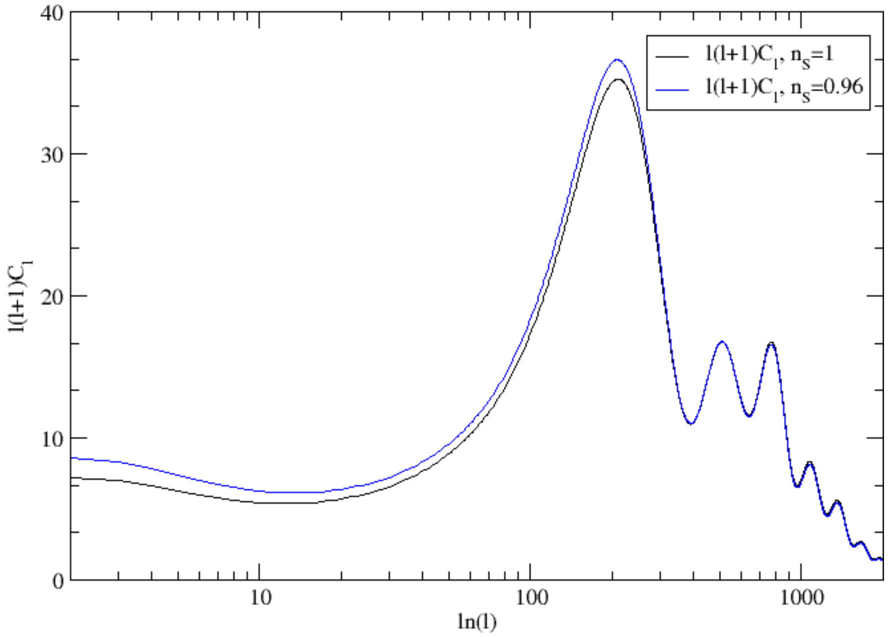

Figure 7.1: The power spectrum for $n_S = 1$ and $n_S = 0.964$, where the latter represents the power spectrum of this model, for arbitrary units.

7.1.2 Results for the Non-Gaussianity Parameter

We'll here analyze which of the configurations are the dominant one. In general the literature seem to imply the equilateral configuration to be the dominant one. As we see from the equations above this does seem to be the case; however it only dominates by approximately 1%. In Figure 7.2 we show the surface $f_{\rm NL}(\beta, \phi)$ for $N = 55$. Also plotted in green is the approximate $f_{\rm NL,approx}$, forming the flat surface beneath. Figure 7.3 shows the fractional error between these, which is defined as

$$\mathrm{Err} = \frac{|\mathrm{f}_{\mathrm{NL,approx}} - \mathrm{f}_{\mathrm{NL}}|}{\mathrm{f}_{\mathrm{NL}}}. \tag{7.16}$$

We can see that the equilateral line (at $\{\beta, \phi\} = \{1, 2\pi/3\}$) is dominant and the squeezed line (at $\{\beta, \phi\} = \{1, \pi\}$) gives the weakest contribution; however, the maximum error in assuming the approximate form is Err $\lesssim 1.6\%$. As $\beta \to \infty$ we can see the f_{NL} parameter in Figure 7.2 decaying towards the squeezed value; this is also very apparent in Figure 7.3. These results do not suggest that we can simply employ $f_{\rm NL}^{\rm Eq}$ in the calculation of the CMB angular bispectrum, since unless there is a mechanism that preferentially selects the equilateral configuration it is not dominant enough, even for low N, that the rest of the parameter space can be neglected.

As we increase the number of e-foldings for inflation we would expect the exact form of the $f_{\rm NL}$ parameter to go to the approximate form. In Figure 7.3 we show the fractional error Err for $N = 55$ and $N = 750$. The lower surface, $N = 750$, is noticeably flatter as

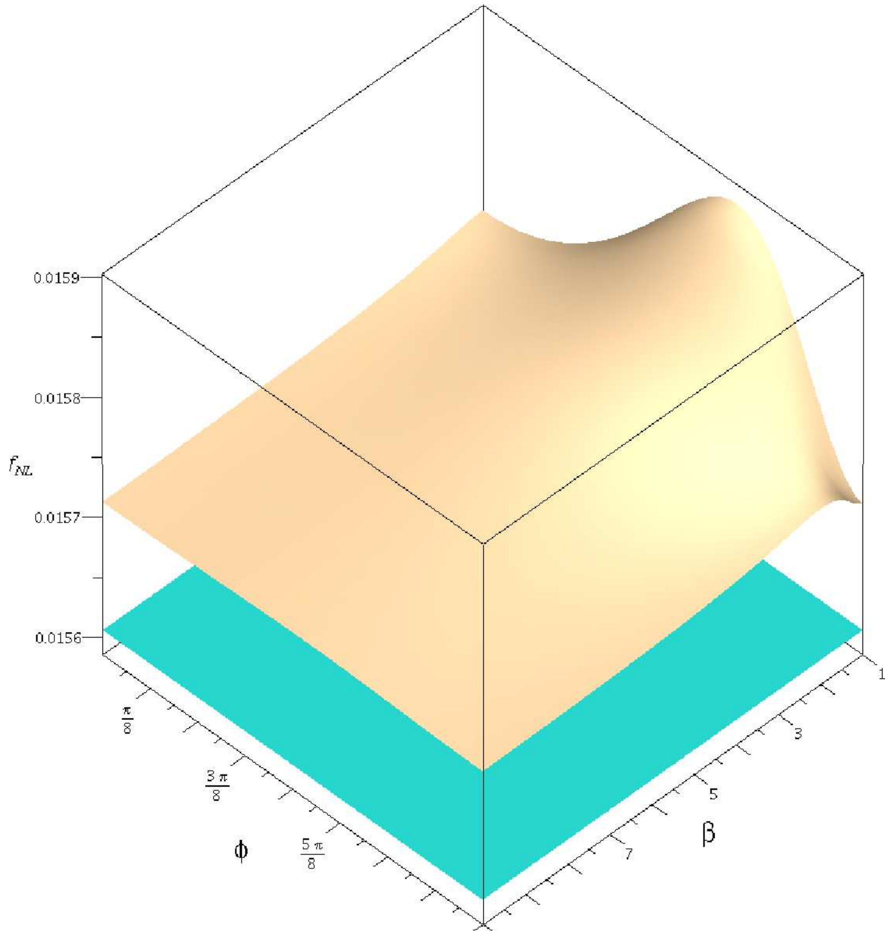

Figure 7.2: $f_{\rm NL}$ (upper curve) and $f_{\rm NL,approx}$ for $N = 55$.

well as having lower fractional errors in general. Pushing to an extremely high N gives effectively vanishing fractional error across the entire plane. This is also illustrated in Figure 7.4, which shows the ratios $f_{\rm NL}^{\rm Eq}/f_{\rm NL}^{\rm Col}$, $f_{\rm NL}^{\rm Eq}/f_{\rm NL}^{\rm Sq}$ and $f_{\rm NL}^{\rm Eq}/f_{\rm NL}(\beta = 9, \phi = 8\pi/10)$. In each case the fractional error decays cleanly with increasing N, and the equilateral line remains the largest.

Alternatively, we can go back to the original definition of $f_{\rm NL}$ (4.29), before we introduced the parametrization, and evaluate a three-dimensional plot of how $f_{\rm NL}$ evolves for all various k-configurations (naturally restricted to a triangular wedge). In Figure 7.5 and Figure 7.6 we show the $f_{\rm NL}$ from two different perspectives, the front and the rear.

7.1.3 Results for the Bispectrum

It turns out that it is possible to calculate an analytical approximation of the reduced angular bispectrum $\hat{B}_{l_1 l_2 l_3}$ (2.130), but only for low $l \leq 20$. This area is named the

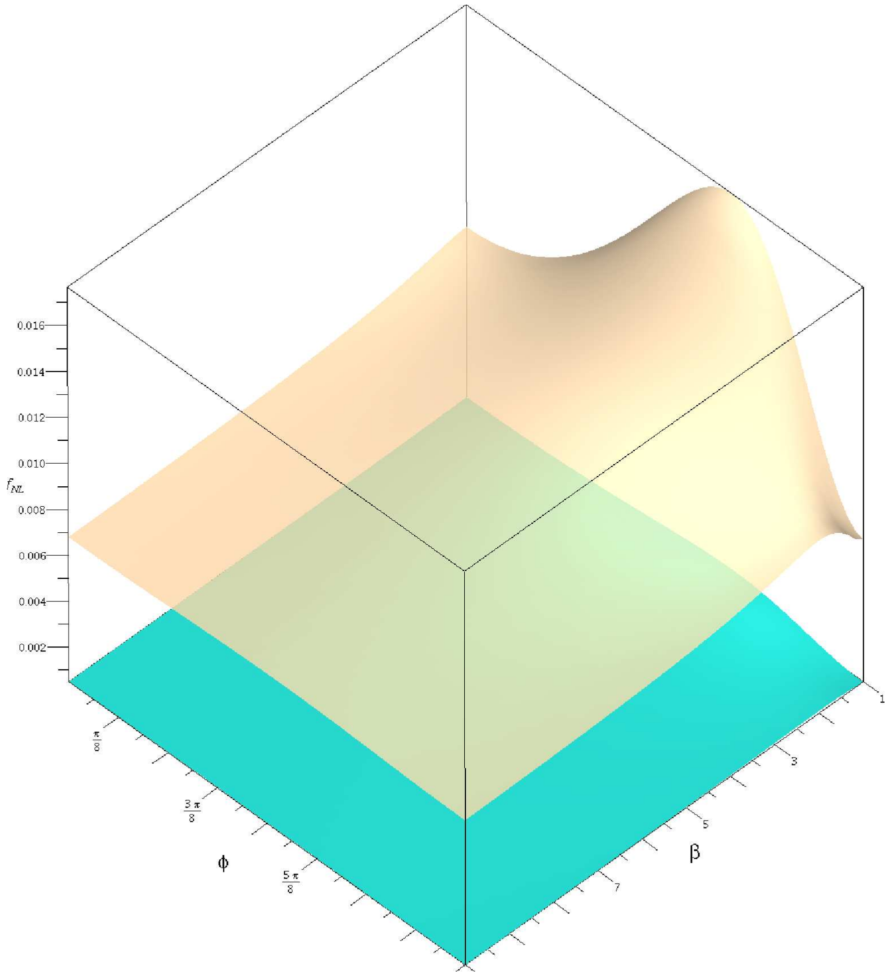

Figure 7.3: Fractional error in $f_{\text{NL,approx}}$ for $N = 55$ (upper) and $N = 750$ (lower).

Sachs-Wolfe plateau in the literature, and our analytical approximation when having chosen $n_S = 1$ is

$$\hat{B}_{l_1 l_2 l_3} \approx -\frac{4\pi^{5/2}}{90} f_{\text{NL}} \frac{1}{l_1(l_1+1)} \frac{1}{l_2(l_2+1)} + 2\text{perms}; \tag{7.17}$$

see Appendix C for the derivation. We choose to look at the equilateral and colinear configurations, $l_1 = l_2 = l_3 = l$ and $l_1 = l_2 = l_3/2 = l$ respectively, in Figure 7.7, where we have also plotted the power spectrum for this model in comparison.

We also present the full solution to this approximation in in Figure 7.8 and Figure 7.9, front and rear perspective respectively, for $l < 20$.

Figure 7.8 and Figure 7.9 shows us the discrete nature of the bispectrum, and we see a clear diminishing of the bispectrum as l increases. Note again that the bispectrum is only defined for l-configurations that form a triangle, and for even ls. Figure 7.7 clearly

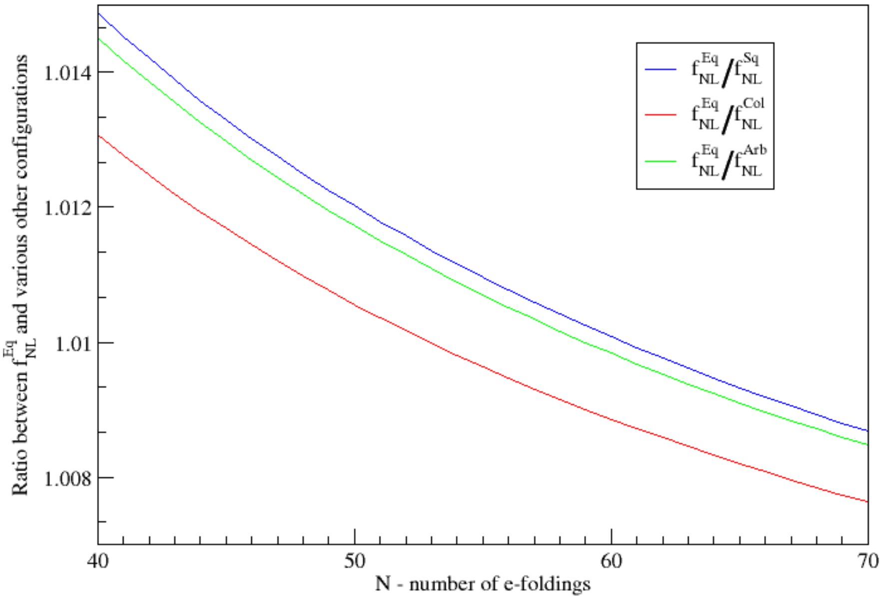

Figure 7.4: Ratios between $f_{\mathrm{NL}}^{\mathrm{Eq}}$ and $f_{\mathrm{NL}}^{\mathrm{Col}}$, $f_{\mathrm{NL}}^{\mathrm{Sq}}$ and an arbitrary line with $\beta = 9$, $\phi = 8\pi/10$ for varying number of e-foldings N.

shows us that there is an extended Sachs-Wolfe plateau, as for this particular model the f_{NL} is relatively constant. It also demonstrates that the current code is able to do the analysis which is needed for the other extended gravity models we wish to examine at a later time.

Note however that there are two reasons for only analyzing the bispectrum for lower ls at the time being. The first is due to an implementation error that has not yet been identified in the current state of the code. The other problem is more substantial, and has been encountered by many who have been working on the bispectrum, notably by Fergusson and Shellard in [112]. As they have pointed out, and I have experienced, the brightness functions start oscillating as k grows, and eventually hit a limit where the value drastically drops, at $k \sim 0.1$, to continue oscillating until $k \sim 1$ where it completely vanishes. This is a problem because it lower the allowed dynamical range we can use in our calculations, and gives us an outright wrong behaviour at high ks. Fergusson and Shellard decided to strip out the source function from the brightness function integral, in order to construct the brightness function manually using the precomputed source function. Depending on stability we might decide to go the same route.

The next step would also be analyze the matter power spectrum $\langle|\delta_M|^2\rangle$ and matter bispectrum $\langle\delta_M\delta_M\delta_M\rangle$, which has so far been neglected.

Finally once we have all of the above running perfectly, we will apply them to the other $f(R)$ theories expanded upon in §3.4. A potentially interesting $f(R)$ model would be a variation of the first alternative theory discussed in §3.4.3, which is already ruled out from the Amendola and Tsjuikawa bounds [54], of the form

$$f(R) = -\frac{\mu^4}{R-r} - 2\Lambda + R - r + \alpha(R-r)^2.$$

This represents a Laurent series that is no longer expanding about the point $R = 0$, but has rather been shifted with a factor r. It seems possible this slight modification might push the theory towards something more viable.

It is worth emphasising that we have used $f(R) = R + \alpha R^2$ because it is the simplest test case, the techniques employed applies to general $f(R)$ theories, to Brans-Dicke theories, and to more general modified gravities. While we don't expect observable bispectra from $f(R)$ the formalism developed will be able to take more general models which may well do. Finally, all the underpinnings are all here, pending testing of the code.

The only thing that now remains is to stabilize the code and complete the implementations of all mentioned $f(R)$ theories, and other interesting extended gravity theories as they are brought to our attention.

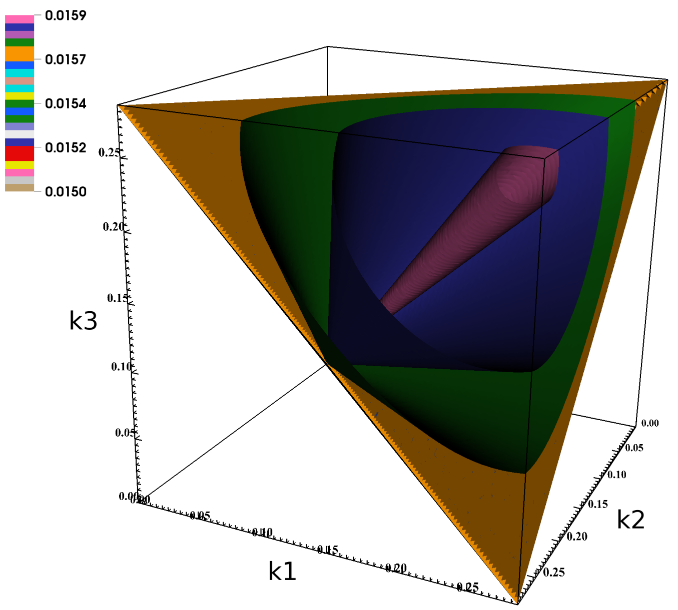

Figure 7.5: The non-linearity parameter $f_{\rm NL}$ for k_1, k_2 and k_3 running from 0 to 25, color scheme is the value of the $f_{\rm NL}$.

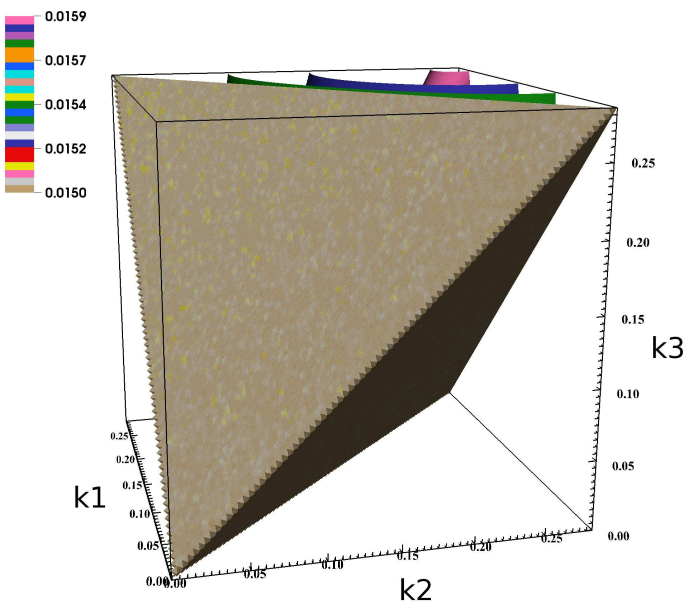

Figure 7.6: Same as the above picture, seen from the opposite side. 3D representation courtesy of supervisor Iain Brown.

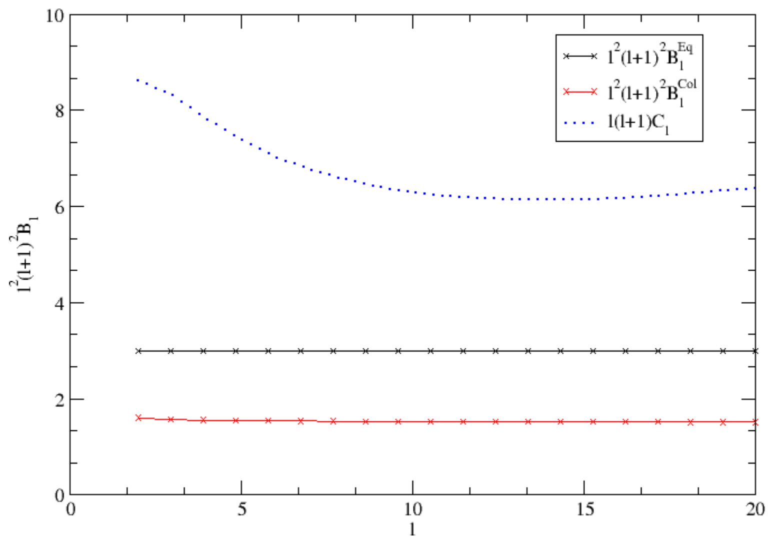

Figure 7.7: The analytical approximation of the reduced angular bispectrum at the Sachs-Wolfe plateau, for arbitrary units. Dotted is the C_l for the same model for comparison, it has been scaled down in order to compare its shape to the bispectrum.

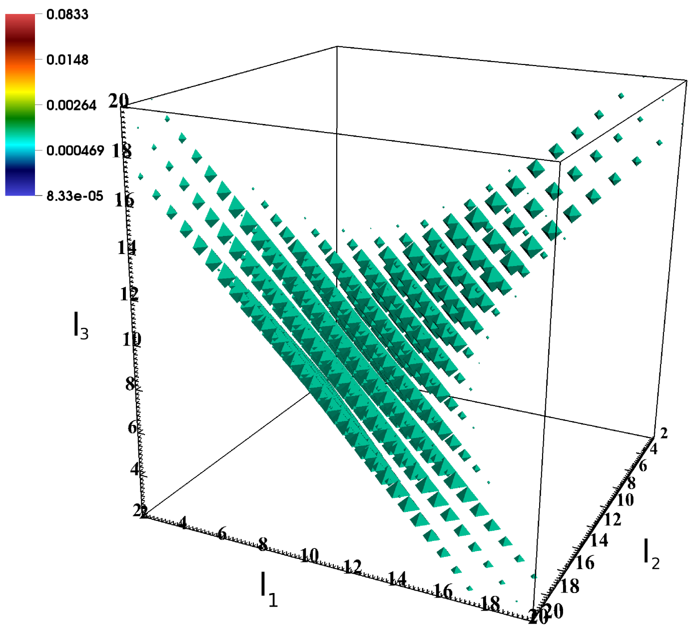

Figure 7.8: The reduced angular bispectrum $\hat{B}_{l_1 l_2 l_3}$.

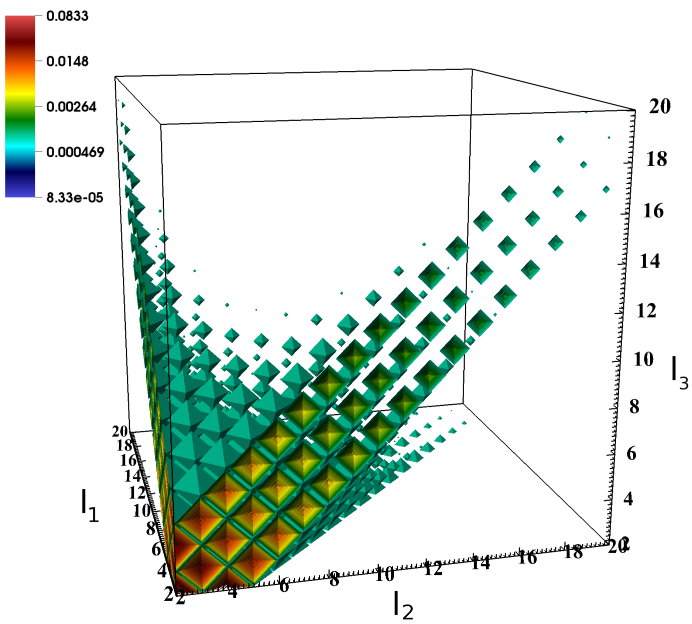

Figure 7.9: Same as the above picture, seen from the opposite side. 3D presentation courtesy of supervisor Iain Brown.

Chapter 8

Conclusions

This thesis has utilized $f(R)$ theories of gravity, most notably the $f(R) = R + \alpha R^2$ Starobinsky model but applicable to other $f(R)$ models, to demonstrate how one can exploit the Einstein frame to simplify calculations, how this transformation into the Einstein frame carries certain risks and how to calculate the statistics and dynamics of $f(R)$ theories. We have also modified the existing Boltzmann code CAMB so that it can be used for a wide range of modified gravity theories, and to safeguard against the errors one can induce from the conformal transformation.

We have worked out the general techniques needed for calculating the non-linearity parameter f_{NL}, CMB power spectrum etc. for a wide range of modified gravity models in our modifications to CAMB. The code is practically finished, but is however still untested. Several alternative theories of gravity have been discussed in this thesis that we will apply the code to. However so far we have only utilized the Starobinsky model, as it is the simplest test case and an extensively studied model.

From Chapter 5 and our paper [1] we have shown that any extended gravity theory that can be transformed into an Einstein frame will induce errors during the transformation if we do not take care of the redundant degrees of freedom that appear. This is only not an issue when we are working within a restricted set of gauges where $\Phi \neq 0$, $\Psi \neq 0$ and $\delta\rho \neq 0$. As well as producing new degrees of freedom, it was shown that the transformation does not preserve adiabaticity, and has the chance of introducing isocurvature in the Einstein frame. We have shown that the errors induced in this way are likely to have the same magnitude as the order of the deviation from standard GR. In our chosen model the deviations are low, and can be considered negligible, when we transform the initial conditions. In principle however, we do not know how big these deviations are for other extended gravity theories and however small the errors might be at the initial conditions, we do not know how much they will compound as the equations are evolved. Care should always be taken.

For our chosen model we have analyzed the non-linearity parameter f_{NL} in order to see if it will have an observable value, and to probe whether a specific configuration of the wavenumbers k will dominate over the others. Of the possible configurations we have focused on the equilateral $f_{\mathrm{NL}}^{\mathrm{Eq}}$, squeezed $f_{\mathrm{NL}}^{\mathrm{Sq}}$ and colinear $f_{\mathrm{NL}}^{\mathrm{Col}}$ configurations.

From the results in §7.1.2 we have shown in detail that the equilateral configuration is the dominant configuration, just as the literature has a tendency to imply. However we do note that it does only dominate by barely 1%. This tells us that we cannot just assume an equilateral configuration when calculating quantities such as the non-linearity parameter, CMB angular power spectrum, the bispectrum and so forth, since unless there is a mechanism that automatically selects the equilateral configuration it is not dominant enough, even for a low number of e-foldings N, that the rest of the parameter space can be neglected. In fact, most of the other configurations tend towards the squeezed limit.

Also in §7.1.2 we noted that the value of the non-linearity parameter is approximately constant for all configurations and also quite small: $f_{\rm NL} \approx 0.015$. This is small enough that it probably can never be measured; the current constraints on the $f_{\rm NL}$ as mentioned in §7.1 are $f_{\rm NL}^{\rm Eq} \in (-214, 266)$ and $f_{\rm NL}^{\rm Sq} \in (-10, 74)$, and even though Planck should tighten this considerably, it seems unlikely that the level of accuracy will ever reach this level of precision. This results in this particular $f(R)$ model not being verifiable through the use of non-Gaussianity probes. Even if the non-linearity parameter is found to be, for example, $f_{\rm NL} \in (5, 15)$ with a 68% confidence level then $f_{\rm NL} \approx 0$ is still within two$-\sigma$.[1]

We've also shown that the bispectrum is proportional to the non-linearity parameter, in Appendix C, and used alongside the small value of $f_{\rm NL}$ we can arrive at the conclusion that the CMB bispectrum is unobservable. From this we can assume that the trispectrum is also unobservable[2] for this model.

This covers the major results of this thesis, and unlike many projects and master theses, I have a clear goal for future work: to continue the modification of CAMB, sorting out any remaining implementation errors and technicalities, and then applying the other $f(R)$ theories discussed in this thesis, and other interesting extended gravity theories as they are brought to our attention, to the code. Keep an eye out for the code and a documentation in the near future.

[1] One-σ is equivalent to a 68% confidence level, two-σ a 95% confidence level and three-σ represents a 99.7% confidence level.

[2] Although the statement isn't correct in principle, we justify it by the fact that we cannot today detect a bispectrum on the CMB, and therefore the possibility of the trispectrum is even fainter.

Appendices

Appendix A

General Statistics for any Metric

Working from a general metric, we can find the Ricci scalar for any of the other metrics used in this thesis to second order,

$$ds^2 = a(\eta)^2 \left(-(1+2\Phi)d\eta^2 + 2B_i d\eta dx^i + (\delta_{ij} + 2C_{ij})dx^i dx^j\right), \tag{A.1}$$

where for scalar, vector and tensor components,

$$B_i = \partial_i B + S_i, \quad \partial^i S_i = 0, \quad C_{ij} = -\Psi\delta_{ij} + \partial_i\partial_j E + \partial_{(i}F_{j)} + \frac{1}{2}h^{(T)}_{ij}. \tag{A.2}$$

See Table A.1 for how to transform this to the various gauges we've employed earlier. With this line element the components of the metric take the form

$$\begin{array}{l|l}
g_{00} = -a^2(1+2\Phi), & -a^2 g^{00} = 1 - 2\Phi + 4\Phi^2 - B^i B_i, \\
g_{0i} = a^2 B_i, & a^2 g^{0i} = B^i - 2\Phi B^i - 2B_j C^{ij}, \\
g_{ij} = a^2\left(\delta_{ij} + 2C_{ij}\right), & a^2 g^{ij} = \delta^{ij} - 2C^{ij} + 4C^{ik}C^j_k - B^i B^j.
\end{array} \tag{A.3}$$

Utilizing the definition of the Christoffel symbols equation (2.9), in combination with the above metric components, we find

$$\Gamma^0_{00} = \mathcal{H} + (1-2\Phi)\dot{\Phi} - (1+3\mathcal{H})B^i B_i + B^i\partial_i\Phi, \tag{A.4}$$

$$\Gamma^0_{0i} = (1-2\Phi)\partial_i\Phi + \mathcal{H}\left((1-2\Phi)B_i - 2B_i C^l_l\right) + \left(\frac{1}{2} + \mathcal{H}\right)B^j C_{ij}, \tag{A.5}$$

$$\begin{aligned}\Gamma^0_{ij} = &-(1-2\Phi)\partial_j B_i + \mathcal{H}((1-2\Phi)(\delta_{ij} + 2C_{ij}) + 4\Phi^2\delta_{ij} - B_i B_j) \\ &+ (1-2\Phi)\dot{C}_{ij} + B^k\partial_j C_{ik} + B^k\partial_i C_{jk} - B^k\partial_k C_{ij},\end{aligned} \tag{A.6}$$

$$\Gamma^k_{00} = B^k + \partial^k\Phi - 2C^{kl}B_l - 2C^{kl}\partial_l\Phi - B^k\dot{\Phi} + \mathcal{H}(2B_l C^{lk} - B^k), \tag{A.7}$$

$$\Gamma^k_{0i} = -B^k\partial_i\Phi + \dot{C}^k_i - 2C^{kl}\dot{C}_{li} + \mathcal{H}(\delta^k_i + B^k B_i), \tag{A.8}$$

$$\begin{aligned}\Gamma^k_{ij} = &\,\partial_j C^k_i + \partial_i C^k_j - \partial^k C_{ij} - 2C^{kl}(\partial_j C_{il} + \partial_i C_{lj} - \partial_l C_{ij}) \\ &+ B^k\partial_j B_i - B^k\dot{C}_{ij} - \mathcal{H}((1-2\Phi)B^k\delta_{ij} - B_j C^k_i + B^k C_{ij}).\end{aligned} \tag{A.9}$$

We then proceed to use these together with equation (2.10) to find the Ricci tensor components. First the time-part,

$$\begin{aligned}
R_{00} =\ & \partial_a B^a - \nabla^2\Phi - 2\partial_a C^{al} B_l - 2C^{al}\partial_a B_l - 2C^{al}\partial_a\partial_l\Phi - 2\partial_a C^{al}\partial_l\Phi \\
& - \partial_a B^a\dot{\Phi} + \mathcal{H}(2\partial_a B_j C^{ja} + 2B_j\partial_a C^{ja} - \partial_a B^a) + \dot{B}^a\partial_a\Phi - \ddot{C} \\
& + 2C^{al}\ddot{C}_{al} + 2\dot{C}^{al}\dot{C}_{al} - \dot{\mathcal{H}}(3 + B^a B_a) - \mathcal{H}\dot{B}^a B_a - \mathcal{H}B^a\dot{B}_a + \dot{\Phi}\dot{C} \\
& + 3\mathcal{H}(1-2\Phi)\dot{\Phi} + \mathcal{H}\left(2B^a\partial_a\Phi + \dot{C} - 2C^{al}\dot{C}_{al} - 9\mathcal{H}B^a B_a - 5B^a B_a\right) \\
& + B^b\partial_a C^a_b + B^b\partial_b C - B^b\partial^a C_{ab} + \partial^b\Phi\partial_a C^a_b + \partial^b\Phi\partial_b C - \partial^b\Phi\partial^a C_{ab} \\
& - \partial_a\Phi B^a - \partial^a\Phi\partial_a\Phi - \mathcal{H}\partial^a\Phi B_a - \dot{C}^a_b\dot{C}^b_a + 2\mathcal{H}(2B^a\partial_a\Phi + 2C^{al}\dot{C}_{al}),
\end{aligned} \tag{A.10}$$

then the mixed part,

$$\begin{aligned}
R_{0i} =\ & \frac{1}{2}\dot{B}^j C_{ij} + \frac{1}{2}B^j\dot{C}_{ij} + \dot{\mathcal{H}}\Big((1-2\Phi)B_i + B^j C_{ij} - 2B_i C^l_l\Big) \\
& + \mathcal{H}((1-2\Phi)\dot{B}_i + \dot{B}^j C_{ij} + B^j\dot{C}_{ij} - \dot{\Phi}B_i - 2\dot{B}_i C - 2B_i\dot{C}) + \partial_a\dot{C}^a_i \\
& - \partial_a B^a\partial_i\Phi - B^a\partial_a\partial_i\Phi - 2\partial_a C^{al}\dot{C}_{il} - 2C^{al}\partial_a\dot{C}_{il} + \mathcal{H}\partial_a B^a B_i + 2\mathcal{H}B^a\partial_a B_i \\
& + 2\mathcal{H}(\partial_i B^l B_l + B^l\partial_i B_l) + \partial_i B^l B_l + B^l\partial_i B_l - \partial_i B^l\partial_l\Phi \\
& - B^l\partial_i\partial_l\Phi + \partial_i B^a\partial_a\Phi + B^a\partial_i\partial_a\Phi - \partial_i\dot{C} + 2\partial_i C^{al}\dot{C}_{al} + 2C^{al}\partial_i\dot{C}_{al} \\
& - \partial_i\Phi(\dot{C} + 4\mathcal{H}) + 3\mathcal{H}\left[\mathcal{H}(B_i + B^j C_{ij} - 2\Phi B_i - 2B_i C) - 2\Phi\partial_i\Phi + \frac{1}{2}B^j C_{ij}\right] \\
& + \mathcal{H}B_i\dot{C} + \dot{C}^b_i(\partial_a C^a_b + \partial_b C - \partial^a C_{ab}) - \dot{C}^b_a(\partial_i C^a_b + \partial_b C^a_i - \partial^a C_{ib}) \\
& - \mathcal{H}\Big[B^a\partial_i B_a + 2\mathcal{H}B_i C\Big] - \mathcal{H}(B_i - 2C^l_i B_l - 2C^l_i\partial_l\Phi - \mathcal{H}B_i)) \\
& + B^b(\partial_i B_b - 2\mathcal{H}C_{bi} - \dot{C}_{bi}) + 2\mathcal{H}\Phi B_i,
\end{aligned} \tag{A.11}$$

and finally the spatial part,

$$\begin{aligned}
R_{ij} =\ & -(1-2\Phi)\partial_j\dot{B}_i - 3\dot{\Phi}\partial_j B_i + \frac{\ddot{a}}{a}((1-2\Phi)(\delta_{ij} + 2C_{ij}) + 4\Phi^2\delta_{ij} - B_j B_i) \\
& + \mathcal{H}((1-2\Phi)2\dot{C}_{ij} - (1-4\Phi)2\dot{\Phi}\delta_{ij} - 4\dot{\Phi}C_{ij} - 4\Phi\dot{C}_{ij} - \dot{B}_j B_i - B_j\dot{B}_i) \\
& + (1-2\Phi)\ddot{C}_{ij} - 2\dot{\Phi}\dot{C}_{ij} + \dot{B}^k\partial_i C_{jk} + B^k\partial_i\dot{C}_{jk} - \dot{B}^k\partial_k C_{ij} - B^k\partial_k\dot{C}_{ij} \\
& + \partial_a\partial_i C^a_j - \nabla^2 C_{ij} - 2\partial_a C^{al}(\partial_i C_{lj} - \partial_l C_{ij}) - 2C^{al}\Big(\partial_a\partial_i C_{lj} - \partial_a\partial_l C_{ij}\Big) \\
& + \partial_a B^a\partial_j B_i - \partial_a B^a\dot{C}_{ij} - B^a\partial_a\dot{C}_{ij} - \mathcal{H}\Big((1-2\Phi)\partial_a B^a\delta_{ij} - 2\partial_a\Phi B^a\delta_{ij} \\
& - 2\partial_a B_j C^a_i - 2B_j\partial_a C^a_i + \partial_a B^a C_{ij}\Big) - (1-2\Phi)\partial_j\partial_i\Phi + \partial_j\Phi\partial_i\Phi \\
& + 2\mathcal{H}(\partial_j B_i C - B_i\partial_j C) + \frac{1}{2}\Big(\partial_j B^l C_{il} + B^l\partial_j C_{il}\Big) - \partial_j\partial_i C + \partial_j\partial^a C_{ia} \\
& + 2\partial_j C^{al}(\partial_i C_{al} - \partial_l C_{ai}) + 2C^{al}(\partial_j\partial_i C_{al} - \partial_j\partial_l C_{ai}) - \partial_j B^a\partial_a B_i
\end{aligned} \tag{A.12}$$

$$
\begin{aligned}
&+\partial_j B^a \dot{C}_{ai} + B^a \partial_j \dot{C}_{ai} - 2\mathcal{H}(\partial_j B_a C^a_i + B_a \partial_j C^a_i) \\
&+\mathcal{H}((1-2\Phi)\dot{\Phi}\delta_{ij} + 2\dot{\Phi}C_{ij}) + \dot{\Phi}\dot{C}_{ij} + \mathcal{H}\Big((1-2\Phi)\dot{C}_{ij} + B^k\partial_j C_{ik} \\
&+B^k\partial_i C_{jk} - B^k\partial_k C_{ij}\Big) - \dot{C}\partial_j B_i + \mathcal{H}(\delta_{ij} + 2C_{ij})\dot{C} + C\dot{C}_{ij} \\
&+2\mathcal{H}B^a\partial_a C_{ij} + \partial_b\Phi(\partial_j C^b_i + \partial_i C^b_j - \partial^b C_{ij} - \mathcal{H}B^b\delta_{ij}) \\
&-\dot{C}^a_j\Big((1+2\mathcal{H})C_{ai} - \partial_i B_a\Big) - (1-2\Phi)\mathcal{H}\dot{C}_{ij} + 2\mathcal{H}C^l_i\dot{C}_{lj} \\
&-\mathcal{H}\Big[-(1-2\Phi)\partial_j B_i - \mathcal{H}((1-2\Phi)(\delta_{ij} + 2C_{ij}) \\
&+4\Phi^2\delta_{ij}) + (1-2\Phi)\dot{C}_{ij} + B^k\partial_j C_{ik} + B^k\partial_i C_{jk}\Big] \\
&-\dot{C}^a_i\Big((1+2\mathcal{H})C_{aj} - \partial_j B_a\Big) - (1-2\Phi)\mathcal{H}\dot{C}_{ij} + 2\mathcal{H}C^l_j\dot{C}_{il} - 5\mathcal{H}^2 B_i B_j \\
&+\partial_b C\Big(\partial_j C^b_i + \partial_i C^b_j - \partial^b C_{ij} - \mathcal{H}B^b\delta_{ij}\Big) + \partial_a C^a_b\Big(\partial_j C^b_i + \partial_i C^b_j - \partial^b C_{ij} - \mathcal{H}B^b\delta ij\Big) \\
&-\partial^a C_{ab}\Big(\partial_j C^b_i + \partial_i C^b_j - \partial^b C_{ij} - \mathcal{H}B^b\delta_{ij}\Big) - \partial_b C^a_j\Big(\partial_a C^b_i + \partial_i C^b_a - \partial^b C_{ai}) \\
&-\partial_j C^a_b\Big(\partial_a C^b_i + \partial_i C^b_a - \partial^b C_{ai}) + \partial^a C_{jb}\Big(\partial_a C^b_i + \partial_i C^b_a - \partial^b C_{ai}\Big).
\end{aligned}
$$

Having all the terms, all we need to do is use equation (2.11) to find the general Ricci scalar for any metric,

$$
R = g^{\mu\nu}R_{\mu\nu} = g^{00}R_{00} + 2g^{0i}R_{0i} + g^{ij}R_{ij}. \tag{A.13}
$$

Due to the nature of our metric components A.3, we see that it would be to our advantage to calculate a^2R rather than just R,

$$
\begin{aligned}
a^2R = (1-2\Phi)&\Big[2\ddot{C} + 3\dot{\mathcal{H}}\Big] + 2\Phi\dot{C} + 6\mathcal{H}\dot{C} \\
&+2\partial_a C^{al}B_l + 2C^{al}\partial_a B_l + 2C^{al}\partial_a\partial_l\Phi + 2\partial_a C^{al}\partial_l\Phi + \partial_a B^a\dot{\Phi} \\
&-4\mathcal{H}(\partial_a B_j C^{ja} + B_j\partial_a C^{ja}) - \dot{B}^a\partial_a\Phi - 2C^{al}\ddot{C}_{al} \\
&-2\dot{C}^{al}\dot{C}_{al} + \mathcal{H}\dot{B}^a B_a + \mathcal{H}B^a\dot{B}_a - \dot{\Phi}\dot{C} + 12\dot{\mathcal{H}}\Phi^2 \\
&-\mathcal{H}\left(2B^a\partial_a\Phi - 2C^{al}\dot{C}_{al} - 5B^a B_a\right) - B^b\partial_a C^a_b - B^b\partial_b C \\
&+2B^i\Big[\mathcal{H}\dot{B}_i + \partial_a\dot{C}^a_i - \partial_i\dot{C} - 4\mathcal{H}\partial_i\Phi - \mathcal{H}B_i\Big] + 5\mathcal{H}^2 B_a B^a \\
&-(1-2\Phi)\partial_b\dot{B}^b - 3\dot{\Phi}\partial_b B^b + 3\frac{\ddot{a}}{a}\left((1-2\Phi) + 4\Phi^2\right) + \frac{\ddot{a}}{a}(2C + B_b B^b) \\
&+\mathcal{H}(-3\dot{\Phi} + 18\Phi\dot{\Phi} - 4\dot{\Phi}C - 8\Phi\dot{C} - 2\dot{B}_b B) \\
&-\dot{\Phi}\dot{C} + \dot{B}^k\partial_b C^b_k + B^k\partial_b\dot{C}^b_k - \dot{B}^k\partial_k C - B^k\partial_k\dot{C} \\
&+2\partial_a\partial^b C^a_b - 2\nabla^2 C - 2\partial_a C^{al}(\partial_b C^b_l - \partial_l C) - 2C^{al}\Big(\partial_a\partial_b C^b_l - \partial_a\partial_l C\Big)
\end{aligned}
$$

$$
\begin{aligned}
&+ \partial_a B^a \partial_b B^b - \partial_a B^a \dot{C} - B^a \partial_a \dot{C} - \mathcal{H}\Big((1-2\Phi)\partial_a B^a \\
&- 2\partial_a B_b C^{ab} - 2B_b \partial_a C^{ab} - \partial_a B^a C\Big) + \partial_b \Phi \partial^b \Phi \\
&- \mathcal{H} B^b \partial_b C + \frac{1}{2}\Big(\partial_b B^l C_l^b + B^l \partial_b C_l^b\Big) + \frac{\ddot{a}}{a}(4C^{ik}C_{ik} - B^i B_i) \\
&+ 2\partial_b C^{al}(\partial^b C_{al} - \partial_l C_a^b) + 2C^{al}(\nabla C_{al} - \partial_b \partial_l C_a^b) - \partial_b B^a \partial_a B^b \\
&+ \partial_b B^a \dot{C}_a^b + B^a \partial_b \dot{C}_a^b + C\dot{C} + \partial_a \Phi(2\partial_b C^{ab} - \partial^a C + 3\mathcal{H} B^a) \\
&- 2\dot{C}^{ab}\Big((1+2\mathcal{H})C_{ab} - \partial_b B_a\Big) + 4\mathcal{H}\Phi\dot{C} + 4\mathcal{H} C_b^l \dot{C}_l^b \\
&- \mathcal{H}\Big[-\mathcal{H}((1-2\Phi)(3+2C) + 12\Phi^2)\Big] - \partial_b C_l^a \partial^b C_a^l + \partial^a C_l^b \partial_b C_a^l \\
&+ \partial_a C\Big(2\partial_b C^{ab} - \partial^a C - 3\mathcal{H} B^a\Big) + \partial_a C_l^a\Big(2\partial_b C^{bl} - \partial^l C - 3\mathcal{H} B^l\Big) \\
&- \partial^a C_{al}\Big(2\partial_b C^{bl} - \partial^l C - 3\mathcal{H} B^l\Big) - \partial_l C^{ab}\Big(\partial_a C_b^l + \partial_b C_a^l - \partial^l C_{ab}) \\
&- 2C^{ij}\Big[-\partial_j \dot{B}_i + \frac{\ddot{a}}{a}(1-2\Phi)\delta_{ij} + 2\frac{\ddot{a}}{a}C_{ij} + 3\mathcal{H}\dot{C}_{ij} - 2\dot{\Phi}\delta_{ij} + \ddot{C}_{ij} \\
&+ \partial_a \partial_i C_j^a - \nabla^2 C_{ij} - \partial_j \partial_i \Phi - \partial_j \partial_i C + \partial_j \partial^a C_{ia} + \mathcal{H}^2(1-2\Phi)\delta_{ij} \\
&+ \mathcal{H}\partial_j B_i - 2\mathcal{H}\dot{C}_{ij} - \mathcal{H} C_{ij}\Big].
\end{aligned}
\tag{A.14}
$$

Here follow a table that tell us how to reduce the above quantities to the various gauges we have used

Table A.1: Gauge transformations

Gauges	Vanishing components
Synchronous	$\Phi_S = B_S = 0$, $C_{ij,S} = \frac{1}{2}h_{ij}$
Conformal Newtonian	$B_N = 0$, $E = 0$, $C_{ij,N} = \Psi\delta_{ij}$
Spatially Flat	$E = 0$, $\Psi = 0$
Uniform Field	$E = 0$
Uniform Density	$E = 0$ or $B = 0$

Note that for the latter three we also need to perform changes to the matter content of the Universe, as detailed in §2.7.6.

Appendix B

Arbitrary $f_{\rm NL}$

We worked out the expression for the non-linearity parameter $f_{\rm NL}$ for an arbitrary configuration, using the angle parametrization of the k-configurations; however due to its convoluted form we present it here instead of in §7.1. We use the expression for the $f_{\rm NL}$ (4.29), equation (4.28) and a quick rewrite of the configuration (7.6) of the form

$$k_2 = \beta k_1, \quad k_3 = \gamma k_1, \tag{B.1}$$

where $\gamma = \sqrt{1+\beta^2+2\beta\cos\phi}$. We then get

$$f_{\rm NL} = \frac{10}{3}\left(D_1 f_{\rm NL}^{D1} + D_2 f_{\rm NL}^{D2} + D_3 f_{\rm NL}^{D3} + D_4 f_{\rm NL}^{D4}\right), \tag{B.2}$$

with

$$f_{\rm NL}^{D1} = \frac{2\beta\gamma(\beta\gamma+\beta+\gamma)+\beta^3+\gamma^3+\beta^2(1+\gamma^3)+\gamma^2(1+\beta^3)}{2(1+\beta^3+\gamma^3)(1+\beta+\gamma)^2}, \quad f_{\rm NL}^{D2} = -1, \tag{B.3}$$

$$f_{\rm NL}^{D3} = \frac{\gamma^2+\beta^2+\gamma^3+\beta^3+\gamma^2\beta^3+\beta^2\gamma^3}{(1+\beta^3+\gamma^3)(1+\beta+\gamma)^2} + \frac{\beta+\gamma+\gamma^2+\beta^2+\beta\gamma^2+\gamma\beta^2}{4(1+\beta^3+\gamma^3)} - \frac{1}{2}, \tag{B.4}$$

$$\begin{aligned} f_{\rm NL}^{D4} = {} & \frac{2(1+\beta^5+\gamma^5-\beta\gamma(\beta+\gamma+\beta\gamma))+\beta^4+\gamma^4+\beta(1+\gamma^4)+\gamma(1+\beta^4)}{2(1+\beta^3+\gamma^3)(1+\beta+\gamma)^2} \\ & - \frac{3(\beta^3+\gamma^3+\beta^2(1+\gamma^3)+\gamma^2(1+\beta^3))}{2(1+\beta^3+\gamma^3)(1+\beta+\gamma)^2}. \end{aligned} \tag{B.5}$$

Appendix C

Analytical Approximation of the Reduced Angular Bispectrum

We find an analytical approximation to the reduced angular bispectrum (2.130) by using the expression for the non-linearity parameter f_{NL} (4.29), following the same procedure as Fergusson and Shellard in [112]. We start by inverting equation (4.29) to isolate the primordial bispectrum $\mathcal{B}$,

$$\mathcal{B}(k_1, k_2, k_3) = \frac{3}{10}(2\pi)^4 f_{\mathrm{NL}}(k_1, k_2, k_3) \left[\frac{\mathcal{P}(k_1)\mathcal{P}(k_2)}{k_1^3 k_2^3} + 2\text{perms}\right]. \tag{C.1}$$

Then choose to work with the constant approximation of $f_{\mathrm{NL}} \approx f_{\mathrm{NL,approx}}$ (7.8) and insert the above into the expression for the reduced angular bispectrum (2.130) so that,

$$\begin{aligned}\hat{B}_{l_1 l_2 l_3} = &\left(\frac{2}{\pi}\right)^3 \frac{3}{10}(2\pi)^4 f_{\mathrm{NL}} \iiiint x^2 (k_1 k_2 k_3)^2 j_{l1}(k_1, x) j_{l2}(k_2, x) j_{l3}(k_3, x) \\ &\times \left[\frac{\mathcal{P}(k_1)\mathcal{P}(k_2)}{k_1^3 k_2^3} + 2\text{perms}\right] \Delta_{l_1}(k_1)\Delta_{l_2}(k_2)\Delta_{l_3}(k_3) dk_1 dk_2 dk_3 dx.\end{aligned} \tag{C.2}$$

We sort these integrals by dependencies,

$$\begin{aligned}\hat{B}_{l_1 l_2 l_3} &= 2^7 \pi \frac{3}{10} f_{\mathrm{NL}} \int_x x^2 \int_{k_1} \mathcal{P}(k_1) j_{l_1}(k_1 x)\Delta_{l_1}(k_1) \frac{dk_1}{k_1} \int_{k_2} \mathcal{P}(k_2) j_{l_2}(k_2 x)\Delta_{l_2}(k_2) \frac{dk_2}{k_2} \\ &\qquad \times \int_{k_3} k_3^2 \, j_{l_3}(k_3 x)\Delta_{l_3}(k_3) \, dk_3 \, dx + 2\text{perms} \\ &= A \int_x x^2 I_{l_1}(x, \eta_0) I_{l_2}(x, \eta_0) C_{l_3}(x, \eta_0) \, dx + 2\text{perms},\end{aligned} \tag{C.3}$$

where

$$A = 2^7 \pi \frac{3}{10} f_{\mathrm{NL}},$$

$$I_l(x,\eta_0) = \int \mathcal{P}(k) j_l(kx)\Delta_l(k)\frac{dk}{k}, \tag{C.4}$$

$$C_{l_3}(x,\eta_0) = \int_{k_3} k_3^2\, j_{l_3}(k_3x)\Delta_{l_3}(k_3)\, dk_3. \tag{C.5}$$

On small scales, $l \leq 20$, we can approximate the transfer functions Δ_l to spherical Bessel functions on the form

$$\Delta_l(k,\eta_0) = -\frac{1}{3} j_l(k(\eta_0 - \eta_{dec})) = -\frac{1}{3} j_l(ky),$$

which we use to rewrite equation (C.5) to

$$C_{l_3}(x,\eta_0) = C_{l_3}(x,y) = -\frac{1}{3}\int_{k_3} k_3^2\, j_{l_3}(k_3x) j_{l_3}(k_3y)\, dk_3. \tag{C.6}$$

Let's note that equation (C.4) is very similar to equation (2.124), so we can say that $I_l(x,\eta_0) \approx C_l$. Now proceed to a handbook of mathematical functions [113] and we find that

$$\delta(x-y) = \frac{xy}{\pi^2}\int_0^\infty k^2 j_l(kx) j_l(ky)\, dk, \tag{C.7}$$

which is only valid for positive x and y. With this we now get C_{l_3} on the form,

$$C_{l_3}(x,y) = -\frac{1}{3}\frac{\pi^2}{xy}\delta(x-y), \tag{C.8}$$

so that we can get rid of all the x-dependencies and the integral over x in equation (C.3), in the manner of,

$$\begin{aligned}\hat{B}_{l_1l_2l_3} &= A\int_x x^2 I_{l_1}(x,\eta_0) I_{l_2}(x,\eta_0)\left(-\frac{1}{3}\frac{\pi^2}{xy}\right)\delta(x-y)\, dx + 2\text{perms} \\ &= -\frac{A\pi^2}{3} I_{l_1}(y,\eta_0) I_{l_2}(y,\eta_0) + 2\text{perms}. \end{aligned} \tag{C.9}$$

Then we see that $\hat{B}_{l_1l_2l_3} \sim C_{l_1}C_{l_2} + 2\text{perms}$, if now $l(l+1)C_l \sim$constant then we can expect $l^2(l+1)^2\hat{B}_{l_1l_2l_3} \sim$const for $l_1 = l_2 = l_3$. In order to solve the two last integrals, remember equation (4.23) which we can invert to find an expression for the $\mathcal{P}(k)$,

$$n_s - 1 = \frac{d\ln\mathcal{P}}{d\ln k} = \frac{kd\mathcal{P}}{\mathcal{P}dk} \Rightarrow \mathcal{P}(k) = k^{n_s-1}, \tag{C.10}$$

allowing us to rewrite equation (C.4) to

$$I_l(y,\eta_0) = \int k^{n_s-2} j_l(ky)\Delta_l(k)\, dk = -\frac{1}{3}\int k^{n_s-2} j_l(ky) j_l(ky)\, dk. \tag{C.11}$$

This is another standard integral, with the solution [113]

$$I_l(y,\eta_0) = -\frac{1}{3}\frac{\sqrt{\pi}}{4}y^{1-n_S}\frac{\Gamma\left(\frac{3-n_s}{2}\right)\Gamma\left(\frac{2l+n_s-1}{2}\right)}{\Gamma\left(\frac{4-n_s}{2}\right)\Gamma\left(\frac{2l+5-n_s}{2}\right)}. \tag{C.12}$$

We now insert this into equation (C.9) to get

$$\hat{B}_{l_1l_2l_3} = -\frac{A\pi^3}{2^4 3^3}y^{2(1-n_S)}\frac{\Gamma\left(\frac{3-n_s}{2}\right)}{\Gamma\left(\frac{4-n_s}{2}\right)}f(l_1,l_2) + 2\text{perms} \tag{C.13}$$

$$= -\frac{2\pi^4}{90}f_{\text{NL}}y^{2(1-n_S)}\frac{\Gamma\left(\frac{3-n_s}{2}\right)}{\Gamma\left(\frac{4-n_s}{2}\right)}f(l_1,l_2) + 2\text{perms} \tag{C.14}$$

where

$$f(l_1,l_2) = \frac{\Gamma\left(\frac{2l_1+n_s-1}{2}\right)}{\Gamma\left(\frac{2l_1+5-n_s}{2}\right)}\frac{\Gamma\left(\frac{2l_2+n_s-1}{2}\right)}{\Gamma\left(\frac{2l_2+5-n_s}{2}\right)}. \tag{C.15}$$

By assuming $n_S = 1$ we get

$$f(l_1,l_2) \approx \frac{1}{2l_1(l_1+1)}\frac{1}{2l_2(l_2+1)}, \tag{C.16}$$

and then

$$\hat{B}_{l_1l_2l_3} \approx -\frac{4\pi^{5/2}}{90}f_{\text{NL}}\frac{1}{l_1(l_1+1)}\frac{1}{l_2(l_2+1)} + 2\text{perms}. \tag{C.17}$$

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